(FILE 'REGISTRY' ENTERED AT 14:36:19 ON 12 NOV 2004) L24 STR

VAR G1=O/S NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC I

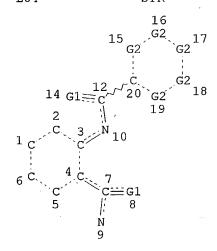
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L26 14784 SEA FILE=REGISTRY SSS FUL L24 — Temp Saved 7 days
L62 STR

VAR G1=O/S
NODE ATTRIBUTES:
NSPEC IS RC AT 9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE L64



VAR G1=O/S VAR G2=N/O/S/CNODE ATTRIBUTES: NSPEC IS RC ATDEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

658 SEA FILE=REGISTRY SUB=L26 SSS FUL (L64 NOT L62) Search for Six 16)

member heterocycles only e

658 ANSWERS "J"

658 ANSWERS "J"

100.0% PROCESSED 14654 ITERATIONS

SEARCH TIME: 00.00.02

FILE 'CAPLUS' ENTERED AT 14:45:28 ON 12 NOV 2004

L69 58 S L65

L70 22 S L69 NOT (PY=>2000 OR PD=>20000322)

E1 THROUGH E56 ASSIGNED

L70 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:699078 CAPLUS

DOCUMENT NUMBER:

131:317778

TITLE: INVENTOR(S):

Phosphate derivatives for treatment of nephritis Miyata, Kazuyoshi; Tsuda, Yoshihiko; Koji, Yasuo; Kuroki, Morihisa; Sakai, Yasuhiro; Mukai, Kiyoshi;

Hashimoto, Kinji; Kori, Hideaki

PATENT ASSIGNEE(S):

Ohtsuka Pharmaceutical Co., Ltd., Japan

Jpn. Kokai Tokkyo Koho, 19 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT:

Searcher :

Shears

571-272-2528

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 11302177	A2	19991102	JP 1998-116645	19980427		
PRIORITY APPLN. INFO.:			JP 1998-116645	19980427		
OTHER SOURCE(S):	MARPAT	131:317778				

Phosphate derivs. (Markush's structures given) are claimed for treatment of nephritis. The derivs. inhibited mesangium cell proliferation in vitro. Examples of tablets, capsules, and granules were formulated.

192723-63-0 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(phosphate derivs. for treatment of nephritis)

192723-63-0 CAPLUS RN

Phosphonic acid, [[5-[[[5-chloro-2-[(methylamino)carbonyl]phenyl]amino]car CN bonyl]pyrazinyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

L70 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:188605 CAPLUS

DOCUMENT NUMBER:

131:340

TITLE:

Reversal of P-glycoprotein mediated multidrug resistance by novel anthranilamide derivatives Roe, Michael; Folkes, Adrian; Ashworth, Philip;

AUTHOR(S):

Brumwell, Julie; Chima, Lal; Hunjan, Sukhjit; Pretswell, Ian; Dangerfield, Wendy; Ryder, Hamish;

Charlton, Peter

CORPORATE SOURCE:

Xenova Ltd., Slough, SL1 4EF, UK

SOURCE:

Bioorganic & Medicinal Chemistry Letters (1999), 9(4),

595-600

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

DOCUMENT TYPE:

Elsevier Science Ltd.

Journal

LANGUAGE: English AB

We have synthesized and evaluated a series of anthranilamide based modulators of P-glycoprotein. These studies have identified XR9576, a potent inhibitor of P-glycoprotein in vitro and in vivo. The general synthesis and the SAR of these compds. are described.

IT 206873-73-6P 206873-74-7P 206873-76-9P

206873-77-0P 206873-78-1P

Searcher : 571-272-2528 Shears

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel anthranilamide derivs. for reversal of

P-glycoprotein

mediated multidrug resistance)

RN 206873-73-6 CAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-74-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-76-9 CAPLUS

CN Pyrazinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

MeO
$$N \rightarrow CH_2 - CH_2$$
 $N \rightarrow CH_2 - CH_2$ $N \rightarrow CH_2 - CH_2$

RN 206873-77-0 CAPLUS

CN Pyrazinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-5-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text$$

RN 206873-78-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-6-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{MeO} \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \end{array}$$

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1998:724208 CAPLUS

DOCUMENT NUMBER:

130:33033

TITLE:

Chromium picolinate complexes and pharmaceuticals with

hypoglycemic or insulin-lowering effect

INVENTOR(S):

Kuroki, Yasuhisa

PATENT ASSIGNEE(S):

Otsuka Pharmaceutical Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

GΙ

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
				-		
JP 10298189	A2	19981110	JP 1997-112682	19970430		
PRIORITY APPLN. INFO.:			JP 1997-112682	19970430		
OTHER SOURCE(S):	MARPAT	130:33033				

AB Hypoglycemic agents, their compns., or insulin-lowering compns. contain Cr complexes I [R1-R3 = H, lower alkyl, OH, benzoyl, lower alkoxycarbonyl, halo-substituted 3-(lower alkyl)-4(3H)-quinazolin-2-yl; R1 = R2 = R3 # H] and optional carriers. 3-Hydroxypicolinic acid (4.17 g) was treated with 2.66 g CrCl3.6H2O in H2O at 80° for 5 h to give 1.67 g trans-I.1/2H2O (R1 = OH, R2 = R3 = H), which was orally administered to dexamethasone-treated rats to show 5% decrease of blood glucose (at 10 mg/kg dose) and 25% decrease of blood insulin (at 100 mg/kg dose). Formulation examples are given.

IT 216656-75-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chromium picolinate complexes as hypoglycemic or insulin-lowering agents)

RN 216656-75-6 CAPLUS

CN 2-Pyridinecarboxylic acid, 5-[[[5-chloro-2-[(methylamino)carbonyl]phenyl]a mino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

L70 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:606819 CAPLUS

DOCUMENT NUMBER: 129:297543

TITLE: Synthesis and structure of chiral 2,6-bis[(2-

carbamoylphenyl)carbamoyl]pyridine ligands

AUTHOR(S): Yu, Qiang; Baroni, Timothy E.; Liable-Sands, Louise;

Rheingold, Arnold L.; Borovik, A. S.

CORPORATE SOURCE: Department of Chemistry, University of Kansas,

Lawrence, KS, 66045, USA

SOURCE: Tetrahedron Letters (1998), 39(38), 6831-6834

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

The synthesis and structure of enantiomerically pure 2,6-bis[(2-carbamoylphenyl)carbamoyl]pyridine ligands are described. Appended from the aryl groups are optically active groups which provide a chiral environment around the planar pyridine core. NMR and x-ray diffraction studies show that these ligands contain helical character which is maintained by a network of intramol. H bonds. These ligands can bind metal ions through their tridentate diamidato-pyridyl chelate to form optically active metal complexes. A Ni complex is prepared and its x-ray crystal structure is determined. The modular design of these ligands offers a

variety of chiral environments about the metal chelate that can be useful in the synthesis of metal reagents for asym. transformations.

IT 214203-39-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with nickel)

RN 214203-39-1 CAPLUS

CN L-Valine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 214203-41-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 214203-41-5 CAPLUS

CN L-Alanine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonyl)]bis-, dimethyl ester, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 214203-38-0 CMF C29 H29 N5 O8

Absolute stereochemistry.

CM 2

CRN 75-09-2 CMF C H2 Cl2

 ${\tt Cl-CH_2-Cl}$

IT 214203-38-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)

RN 214203-38-0 CAPLUS

CN L-Alanine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 214203-40-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 214203-40-4 CAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[[[(1S)-1-phenylethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1998:13933 CAPLUS

DOCUMENT NUMBER:

128:75193

TITLE:

Preparation of aminophthalic acid derivatives as

pesticides.

INVENTOR(S):

Elbe, Hans-Ludwig; Dutzmann, Stefan; Stenzel, Klaus

PATENT ASSIGNEE(S):

Bayer Aktiengesellschaft, Germany

SOURCE:

PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE			
WO 9747589	A1 19971218	WO 1997-EP2845	19970602			
	BR, BY, CA, CN,	CZ, HU, IL, JP, KR, KZ,	LK, MX, NO,			
NZ, PL, RO,	RU, SK, TR, UA,	US				
RW: AT, BE, CH,	DE, DK, ES, FI,	FR, GB, GR, IE, IT, LU,	MC, NL, PT,			
SE, BF, BJ,	CF, CG, CI, CM,	GA, GN, ML, MR, NE, SN,	TD, TG			
DE 19623744	A1 19971218	DE 1996-19623744	19960614			
AU 9730936	A1 19980107	AU 1997-30936	19970602			
PRIORITY APPLN. INFO.:		DE 1996-19623744	19960614			
		WO 1997-EP2845	19970602			
OTHER SOURCE (S) .	MARPAT 128.7519	٠				

OTHER SOURCE(S):

MARPAT 128:75193

GI

Use of title compds. [I; Q1, Q2 = 0, S; R1 = H, R11CO; R2 = R8R9NCO, AΒ R100CO, R11CO, R12SO2; R8 = H, alkyl, cycloalkyl, (substituted) aryl, heteroaryl; R9 = H, alkyl; R8R9N = (substituted) heterocyclyl; R10 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl; R11 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, aralkyl, heterocyclyl; R12 = alkyl, aryl, heterocyclyl; R1R2 = CR13R14; R1R2N = (substituted) heterocyclyl; R13 = H, alkyl, alkenyl, cycloalkyl, (substituted) aryl, heterocyclyl; R14 = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heterocyclyl, alkoxy, dialkylamino; R13R14 = cycloalkylidene; R3, R4 = OH, alkoxy, alkenyloxy, alkynyloxy, aralkoxy, cycloalkoxy, cycloalkenyloxy, aryloxy, heterocyclyloxy, aralkylthio, SH, arylthio, amino, etc.; R5-R7 = H, halo, cyano, NO2, alkyl, alkoxy, alkylthio, haloalkyl, haloalkoxy, haloalkylthio] for combating pests is claimed. Thus, 3-nitrophthalic anhydride was heated with BuOH to give 88.1% 3-nitrophthalic acid 2-Bu ester. The latter was refluxed with DMF di-Me acetal in PhMe to give 92% 3-nitrophthalic acid 1-Me ester 2-Bu

Shears

Searcher :

571-272-2528

ester. This in H2O/THF was treated with Zn and HCl to give 82.4% 3-aminophthalic acid 1-Me ester 2-Bu ester. I at 100 ppm gave 82-98% control of Botrytis cinerea on beans.

IT 200709-28-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aminophthalic acid derivs. as pesticides)

RN 200709-28-0 CAPLUS

CN Benzoic acid, 3-[[(6-chloro-3-pyridinyl)carbonyl]amino]-2-[(methylamino)carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

L70 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1997:667205 CAPLUS

DOCUMENT NUMBER:

127:262339

TITLE:

Novel Folding Patterns in a Family of

Oligoanthranilamides: Non-Peptide Oligomers That Form

Extended Helical Secondary Structures

AUTHOR(S):

Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew

D.

CORPORATE SOURCE:

Department of Chemistry, University of Pittsburgh,

Pittsburgh, PA, 15260, USA

SOURCE:

Journal of the American Chemical Society (1997),

119(44), 10587-10593

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Anthranilamide derivs. are used as the basis for a series of novel oligomers that fold into helical secondary structures in the solid state. When combined with pyridine-2,6-dicarboxylic acid and 4,6-dimethoxy-1,3-diaminobenzene subunits, oligoanthranilamides can be induced to take up a coiled conformation corresponding to two turns of a helix. X-ray crystallog, show that intramol, hydrogen bonding and π - π stacking interactions are important in stabilizing the extended helical structures. Furthermore, both exptl. and calculated 1H NMR methods indicate that related conformations are taken up by the oligomers in chloroform solution

IT 196312-02-4P 196312-04-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystallog.; helical conformation of oligoanthranilamides)

RN 196312-02-4 CAPLUS

CN Benzoic acid, 2,2'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenyleneiminocarbonyl-6,2-pyridinediylcarbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 196312-04-6 CAPLUS

CN Benzoic acid, 2,2'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenyleneiminocarbonyl-6,2-pyridinediylcarbonylimino-2,1-phenylenecarbonylimino)]bis-, dihexyl_ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

IT 155138-99-1

RL: PRP (Properties)

(helical conformation of oligoanthranilamides)

RN 155138-99-1 CAPLUS

CN Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

IT 196311-73-6P 196311-77-0P 196311-92-9P 196311-95-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of oligoanthranilamides)

RN 196311-73-6 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-(methoxycarbonyl)phenyl]amino]carbonyl]phenyl]amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 196311-77-0 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-(methoxycarbonyl)phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 196311-92-9 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-[(hexyloxy)carbonyl]phenyl]amino]carbonyl]phenyl]amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 196311-95-2 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-[(hexyloxy)carbonyl]phenyl]amino]carbonyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & O & O \\
O & C & O \\
NH & CO_2H
\end{array}$$

$$Me^{-(CH_2)} = O - C & O$$

IT 196312-07-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (model; helical conformation of oligoanthranilamides)

RN 196312-07-9 CAPLUS

CN 2-Pyridinecarboxamide, N,N'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenylene)]bis-(9CI) (CA INDEX NAME)

L70 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1996:446492 CAPLUS

DOCUMENT NUMBER:

125:167496

TITLE:

Oligoanthranilamides. Non-Peptide Subunits That Show

Formation of Specific Secondary Structure

AUTHOR(S):

Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew

р.

CORPORATE SOURCE:

Department of Chemistry, University of Pittsburgh,

Pittsburgh, PA, 15260, USA

SOURCE:

Journal of the American Chemical Society (1996),

118(32), 7529-7541

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB A family of novel oligomers based on the anthranilamide nucleus has been prepared and shown to form well-defined secondary structural features. H NMR and X-ray crystallog, techniques have demonstrated that intramol, hydrogen bonds play a key role in stabilizing both linear sheet and helical conformational forms. An example compound is the oligomeric anthranilamide I.

Ι

IT 155138-99-1P 155139-01-8P 180133-05-5P 180133-06-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and secondary structure determination of oligomeric anthranilamides)

RN 155138-99-1 CAPLUS

CN Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 155139-01-8 CAPLUS

CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-

phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 180133-05-5 CAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[(phenylamino)carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 180133-06-6 CAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[(phenylamino)carbonyl]phenyl]-, 1-oxide (9CI) (CA INDEX NAME)

L70 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:995215 CAPLUS

DOCUMENT NUMBER:

124:117098

TITLE:

Preparation of pyridylanilide derivatives as

fungicides

INVENTOR(S):

Riordan, Peter Dominic; Boddy, Ian Kenneth; Osbourn,

Susan Elisabeth

PATENT ASSIGNEE(S):

Agrevo UK Ltd., UK

SOURCE:

PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

1

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	PATENT NO.			KIND DATE			APPLICATION NO.						DATE				
WO	9525723 A1			19950928 WO 1995-GB570			0		19950316								
	W:	AU,	BG,	BR,	CA,	CN,	CZ,	FI,	HU,	JP,	KR,	KZ,	MX,	NO,	NZ,	PL,	RO,
		RU,	SD,	SK,	UA,	US											
	RW:	ΚE,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,
		LU,	MC,	ΝL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,	MR,	ΝE,
			TD,														
AU	9518	981			A1		1995	1009		AU 1	995-	1898	1		1	9950	316
AU	6884						1998						•				
	7506									EP 1	995-	9114	03		1	9950	316
EP	7506						1998										
		AT,	BE,	CH,	DE,												
CN	1143				Α		1997				995-						
	7477						1997	0228		HŲ 1	996-	2547			1	9950	316
	2142						1998										
BR	9507	105			A		1997				995-				_	9950	
	0951						1997				995-				_	9950	
	1680						1998				995-					9950	
	9502	_					1995				995-					9950	
US	5756	524			Α		1998	0526		US 1	996-	7141	49		1	9960	918

PRIORITY APPLN. INFO.:

GB 1994-5347 WO 1995-GB570 19940318 19950316

OTHER SOURCE(S):

MARPAT 124:117098

GI C

$$\mathbb{R}^{2}$$

$$\mathbb{R}^{2}$$

$$\mathbb{R}^{3}$$

AB Title compds. I [X = 0, S; R1, R2 = H, alkyl, cycloalkyl, alkenyl, etc.; R3 = (substituted) pyridyl, pyrimidinyl, pyrazinyl, etc.] were prepared Condensation of 6-methoxynicotinoyl chloride with Me anthranilate in the presence of Et3N in THF afforded I (X = O; R1 = R2 = H; R3 = 6-methoxy-3-pyridyl) which showed activity against barley powdery mildew, rice blast and apple scab at ≤ 500 ppm.

IT 173055-91-9P 173056-05-8P 173056-17-2P 173056-21-8P 173056-46-7P 173056-75-2P 173056-88-7P 173056-95-6P 173056-96-7P 173056-97-8P 173057-04-0P 173057-19-7P

Ι

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of anilide derivs. as fungicides)

RN 173055-91-9 CAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxyamino)carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 173056-05-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxymethylamino)carbonyl]phenyl]-N-methyl- (9CI) (CA INDEX NAME)

Searcher :

Shears

571-272-2528

RN 173056-17-2 CAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxymethylamino)carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 173056-21-8 CAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[[(phenylmethyl)amino]carbonyl]pheny l]- (9CI) (CA INDEX NAME)

RN 173056-46-7 CAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methylamino)carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 173056-75-2 CAPLUS

CN Carbamic acid, [2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 173056-88-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]-6-methoxy- (9CI) (CA INDEX NAME)

MeO
$$H_2N-C$$
 $C-NH$ O

RN 173056-95-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[(diethylamino)carbonyl]phenyl]-6-methoxy-(9CI) (CA INDEX NAME)

RN 173056-96-7 CAPLUS

CN Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, hydrazide (9CI) (CA INDEX NAME)

RN 173056-97-8 CAPLUS

CN Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, (1-methylethylidene)hydrazide (9CI) (CA INDEX NAME)

RN 173057-04-0 CAPLUS

CN Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, 2-acetylhydrazide (9CI) (CA INDEX NAME)

RN 173057-19-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(4-chlorophenyl)amino]carbonyl]phenyl]-6-methoxy- (9CI) (CA INDEX NAME)

L70 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:915317 CAPLUS

DOCUMENT NUMBER:

124:145557

TITLE:

Structure-based design of achiral anthranilamides as P2/P2' surrogates for symmetry-based HIV protease inhibitors: design, synthesis, x-ray structure, enzyme

inhibition and antiviral activity

AUTHOR(S):

Randad, Ramnarayan S.; Lubkowska, Lucyna; Bujacz, Anna; Naik, Rajan H.; Gulnik, Sergei V.; Yu, Betty; Silva, Abelardo; Munshi, Sanjeev; Lynch, Tracy M.; et al.

CORPORATE SOURCE:

Structural Biochem. Program, Natl. Cancer Inst.-Frederick Cancer Res. Development Center,

Frederick, MD, 21702, USA

SOURCE:

Bioorganic & Medicinal Chemistry Letters (1995),

5(21), 2557-62

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: DOCUMENT TYPE: Elsevier Journal

LANGUAGE:

English

Guided by the structure of HIV PR complexed with 2S,3R,4S,5S-2,5-bis[N,N'-AΒ ((3-hydroxy-2-methylphenyl)carbonyl)amino]-3,4-dihydroxy-1,6-

diphenylhexane, a novel, achiral, non-peptidic anthranil (Ant) group was designed as a P2/P2' ligand. Symmetry-based inhibitors containing

N-(2-pyridinylmethoxycarbonyl) anthranil group are potent antiviral agents.

IT173094-25-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(structure-based design of achiral anthranilamides as P2/P2' surrogates for symmetry-based HIV protease inhibitors)

173094-25-2 CAPLUS RN

L-Altritol, 1,2,5,6-tetradeoxy-2,5-bis[[2-[[(5-CN

methylpyrazinyl)carbonyl]amino]benzoyl]amino]-1,6-diphenyl- (9CI) INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

Me

L70 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:858623 CAPLUS

DOCUMENT NUMBER:

123:256357

TITLE:

Preparation of anthranilic acid amide derivative as cyclic guanosine monophosphate-phosphodiesterase

Searcher :

Shears

571-272-2528

inhibitors

Ozaki, Fumihiro; Ishibashi, Keiji; Ikuta, Hironori; INVENTOR(S):

Ishihara, Hiroki; Souda, Shigeru

PATENT ASSIGNEE(S):

Japan

SOURCE:

PCT Int. Appl., 204 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE WO 9518097 A119950706 WO 1994-JP2262 19941227 W: AU, CA, CN, FI, HU, KR, NO, NZ, RU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE CA 2155662 AA 19950706 CA 1994-2155662 19941227 AU 9512824 Α1 19950717 AU 1995-12824 19941227 B2 19980723 AU 694465 EP 686625 A1 19951213 EP 1995-903999 19941227 EP 686625 В1 19990526 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE 19960313 CN 1994-191311 19941227 CN 1118595 A 19941227 JP 08188563 A2 19960723 JP 1994-336920 HU 74450 A2 19961230 HU 1995-2512 19941227 RU 1995-120194 RU 2128644 C1 19990410 19941227 AT 1995-903999 AT 180468 E 19990615 19941227 19951019 19951025 FI 9503968 . A. FI 1995-3968 19950823 NO 9503305 Α NO 1995-3305 19950823 US 5716993 19980210 US 1995-507476 19950914 Α PRIORITY APPLN. INFO.: JP 1993-347092 A 19931227 JP 1994-299110 A 19941109 WO 1994-JP2262

W 19941227

OTHER SOURCE(S):

MARPAT 123:256357

GΙ

Anthranilamide derivs. [I; R1, R2, R3, R4 = H, halo, OH, (halo)alkyl, (halo)alkoxy, nitro, hydroxyalkyl, cyano, (CH2)pNR9R10, S(O)qR13, (un)protected CO2H, (un)substituted tetrazolyl, CONH2, pyrazolyl, or imidazolyl; or adjacent two substituents selected from R1 - R4 together with the C atoms bonded to them forms a ring; wherein R9, R10 = H, (halo)alkyl, arylalkyl, heteroarylalkyl, acyl, (un)protected CO2H; or NR9R10 forms a ring; p = 0, 1-6; R13 = H, (halo)alkyl; q = 0, 1-2; R5, R6 = H, halo, OH, cyano, (halo)alkyl, (halo)alkoxy; or R5 and R6 together with the C atoms bonded to them form cycloalkane, oxolane, 1,3-dioxolane, or 1,4-dioxane ring; W = N, CH; R7, R8 = H, (halo)alkyl; or R1 and R7 together with the C atoms bonded to them form a ring optionally containing other N, O, or S atom; A = H, (halo)alkyl, X(CH2)mZ; wherein X = CO, CS, CH2, SO2; Z = OH, (halo)alkoxy, cyano, halo, etc.; Y = O, S; n = 0, 1-6] or pharmacol. acceptable salts thereof are prepared These compds. are useful for the treatment of ischemic heart disease, angina pectoris,

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

hypertension, pulmonary hypertension, heart failure, and asthma. Thus, 2-nitro-5-chlorobenzoic acid was refluxed with SOCl2 in benzene for 4 h and concentrated to give 2-nitro-5-chlorobenzoyl chloride which was amidated with piperonylamine in the presence of Et3N in THF to give a benzamide (II; R = NO2). This compound was reduced by Fe powder in a mixture of AcOH,

H2O, and MeOH under gentle refluxing to give, after concentration and treatment

with concentrated HCl in EtOH, N-piperonylanthranilamide derivative II. HCl $\langle \, R \, = \,$

 $\ensuremath{\text{NH2}}\xspace$. An anthranilamide derivative (III) showed IC50 of 0.4 nM against cyclic

guanosine monophosphate-phosphodiesterase preparation from pig aorta.

IT 169043-36-1P 169043-37-2P 169044-06-8P 169044-07-9P 169044-08-0P 169044-09-1P

169044-10-4P 169044-11-5P 169044-56-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors)

RN 169043-36-1 CAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-chlorophenyl]- (9CI) (CA INDEX NAME)

RN 169043-37-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-chlorophenyl]- (9CI) (CA INDEX NAME)

RN 169044-06-8 CAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]-4-cyanophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 169044-07-9 CAPLUS

CN 4-Pyridinecarboxamide, N-[4-bromo-2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 169044-08-0 CAPLUS

CN 4-Pyridinecarboxamide, N-[4-bromo-2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN 169044-09-1 CAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]-4-cyano-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN 169044-10-4 CAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromo-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN 169044-11-5 CAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromophenyl]- (9CI) (CA INDEX NAME)

RN 169044-56-8 CAPLUS

CN 4-Pyridinecarboxamide, N-[5-amino-2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Br & O \\ C-NH-CH_2 & O \\ NH & C \\ O & N \end{array}$$

L70 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:841957 CAPLUS

DOCUMENT NUMBER:

123:339482

TITLE:

Synthesis of boxazomycin B and related analogs

AUTHOR(S):

Suto, Mark J.; Turner, William R.

CORPORATE SOURCE:

Parke-Davis Pharm. Res. Div., Warner Lambert Co., Ann

Arbor, MI, 48105, USA

SOURCE:

Tetrahedron Letters (1995), 36(40), 7213-16

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: DOCUMENT TYPE:

Elsevier Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 123:339482

AB The total synthesis of the novel antibacterial agent boxazomycin B is reported. The synthesis proceeds through a highly functionalized benzene ring in which the key functionalities are introduced early in the synthesis and serve as protecting groups for addnl. transformations.

IT 171010-53-0P 171010-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of boxazomycin B and analogs)

RN 171010-53-0 CAPLUS

CN 4-Pyrimidinecarboxamide, N-[6-(aminocarbonyl)-2-hydroxy-3-methylphenyl]-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

RN 171010-58-5 CAPLUS

CN 4-Pyrimidinecarboxamide, N-[2-(aminocarbonyl)-3,6-dihydroxy-5-methylphenyl]-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{Me} \\ \text{O} & \text{HO} \\ \text{O} & \text{OH} \\ \text{OMe} & \text{C-NH}_2 \\ \text{O} \end{array}$$

L70 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:746792 CAPLUS

DOCUMENT NUMBER:

123:132021

TITLE:

Discovery of Potent Cyclic GMP Phosphodiesterase Inhibitors. 2-Pyridyl- and 2-Imidazolylquinazolines

Possessing Cyclic GMP Phosphodiesterase and Thromboxane Synthesis Inhibitory Activities

AUTHOR(S):

Lee, Sung J.; Konishi, Yoshitaka; Yu, Dingwei T.; Miskowski, Tamara A.; Riviello, Christopher M.; Macina, Orest T.; Frierson, Manton R.; Kondo, Kigen;

Sugitani, Masafumi; et al.

CORPORATE SOURCE:

Biofor Inc., Waverly, PA, 18471, USA

SOURCE:

Journal of Medicinal Chemistry (1995), 38(18), 3547-57

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Moderate cyclic GMP phosphodiesterase (cGMP-PDE, PDE V) inhibitor 2-phenyl-4-anilinoquinazoline (I) was identified utilizing MultiCASE assisted drug design (MCADD) technol. Modification of I was conducted at the 2-, 4-, and 6-positions of the quinazoline ring for enhancement of cGMP-PDE inhibitory activity. The 6-substituted 2-(imidazol-1yl)quinazolines are 1000 times more potent in in vitro PDE V enzyme assay than the well-known inhibitor zaprinast. The 6-substituted derivs. of 2-(3-pyridyl)quinazoline and 2-(imidazol-1-yl)quinazoline exhibited more than 1000-fold selectivity for PDE V over the other four PDE isoenzymes. In addition, 3 cGMP-PDE inhibitors were found to have an addnl. property of thromboxane synthesis inhibitory activity.

IT 157864-28-3P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyridyl- and imidazolylquinazolines as cyclic GMP phosphodiesterase and thromboxane synthesis inhibitors)

RN 157864-28-3 CAPLUS

3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME) CN

> 571-272-2528 Searcher : Shears

L70 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:714439 CAPLUS

DOCUMENT NUMBER:

123:216778

TITLE:

Metallohelices: Effects of Weak Interactions on

Helical Morphology

AUTHOR(S):

Kawamoto, Tatsuya; Prakash, Om; Ostrander, Robert;

Rheingold, Arnold L.; Borovik, A. S.

CORPORATE SOURCE:

Department of Chemistry, Kansas State University,

Manhattan, KS, 66506, USA

SOURCE:

Inorganic Chemistry (1995), 34(17), 4294-5

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER:

American Chemical Society

DOCUMENT TYPE: LANGUAGE:

Journal English

The significant effects of weak interactions on the morphol. of AB metallohelices are demonstrated in metal complexes of the helical ligand 2,6-bis[{(N'-acetophenoyl)anthranilamide}carboxyamide]pyridine (H2L). This ligand contains 2 aryl arrays that are held rigid through hydrogen bonds and covalently attached to a pyridyl diamidate metal binding chelate. The morphologies helixes formed with H2L results from the weak interactions between the appended arrays and the tridentate chelate. H2L has a helical structure in the solid state with the 2 appendage crossing, interacting through π -stacking: (P.hivin.1, a 7.3507(8), b 10.627(1), and c 20.098(3) Å; α 96.64(1), β 98.07(1), γ 90.26(1)°; V = 1543.6(3) Å3, Z = 2, 3598 unique data (Fo $\geq 4\sigma Fo$), R(Rw) = 0.0523(0.0656)). NMR and IR studies on the diamagnetic NiL complex show that the helical structure is present in solution Structural studies by x-ray diffraction methods on the copper(II) derivs. of L2- show the large effects that coordination changes have on helical morphol. Two structural isomers were isolated for CuL: a five coordinate green compound (CuLg) and a four coordinate red complex (CuLr). The five coordinate green complex crystallized from toluene in the space

group

P.hivin.1 with two independent mols. in the asym. unit cell. The unit cell consts. are a 12.402(3), b 15.382(3), and c 23.267(5) Å, α 107.09(2), β 90.68(2), γ 104.18(2)°; V = 4096.4(15) Å3, and Z = 4. Final residuals for the refinement of 985 parameters against 9210 data were R = 0.0678 and Rw = 0.0681 with a GOF = 1.96. The four coordinate red complex crystallized from toluene in the space group

C2/c

with unit cell consts. a 24.087(6), b 12.165(3), and c 23.806 Å; β 117.450(2)°, and Z = 8. Final residuals for the refinement of 442 parameters against 2662 data R = 0.0411 and Rw = 0.0486 with a GOF = 0.95. The differences in these two structural isomers is even more

pronounced in their crystal lattices where micropores dominate the lattice architecture for CuLg and extended helixes are present in CuLr.

IT 168284-90-0

> RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (crystal structure and complexation with copper and nickel)

168284-90-0 CAPLUS RN

2,6-Pyridinedicarboxamide, N,N'-bis[2-[[(2-acetylphenyl)amino]carbonyl]phe CN nyl]- (9CI) (CA INDEX NAME)

L70 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

1995:71053 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 122:105008

Intra- and intermolecular hydrogen bonding control of TITLE:

supramolecular structure

Hamilton, Andrew D.; Hamuro, Yoshitomo; Yang, Ji; AUTHOR(S):

Geib, Steven J.; Fan, Erkang

Department Chemistry, University Pittsburgh, CORPORATE SOURCE:

Pittsburgh, PA, 15260, USA

NATO ASI Series, Series C: Mathematical and Physical SOURCE:

Sciences (1994), 426(COMPUTATIONAL APPROACHES IN

SUPRAMOLECULAR CHEMISTRY), 101-8

CODEN: NSCSDW; ISSN: 0258-2023

Journal DOCUMENT TYPE: English

LANGUAGE: Hydrogen bonding is used to control supramol. structure in two distinct ways. The first involves intramol. hydrogen bonds to stabilize linear and

helical conformations in synthetic oligomers. The second uses intermol. hydrogen bonding to direct the self-assembly of several interacting

subunits.

IT 155138-99-1P 155139-01-8P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystallog. of)

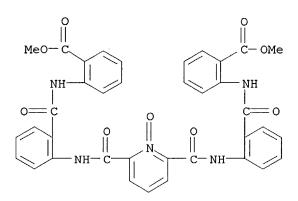
155138-99-1 CAPLUS RN

Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-CN

phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 155139-01-8 CAPLUS

CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



L70 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:620104 CAPLUS

DOCUMENT NUMBER: 121:220104

TITLE: Transition metal complexes of N-(2-benzamide)pyridine-

2'-carboxamide, a potentially tridentate ligand

containing one secondary and one primary amide group: preparation and characterization in the solid state Manessi-Zoupa, E.; Perlepes, S. P.; Hondrellis, V.;

AUTHOR(S): Manessi-Zoupa, E Tsangaris, J. M.

CORPORATE SOURCE: Dep. Chem., Univ. Patras, Patras, Greece

SOURCE: Journal of Inorganic Biochemistry (1994), 55(3),

217-33

CODEN: JIBIDJ; ISSN: 0162-0134

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of N-(2-carbamoylphenyl) pyridine-2-carboxamide (LH2) is reported along with its employment as a ligand. [MCl2(LH2)2].DMF (M = Co,

Ni), [Cu2Cl4(LH2)2].DMF, [CuCl2(LH2)2], [Co(OH)(LH)]n.nH2O, [M2(OH)2(H2O)x(LH)2] (M = Ni, Cu; x = 4, 2), [M(LH)2].xH2O (M = Ni, Cu; x = 0, 1), [Ni(H2O)2(LH)2].H2O, and [CuCl(LH)]n were isolated. The complexes were characterized by elemental analyses, conductivity measurements,

x-ray powder patterns, thermal methods, variable-temperature magnetic susceptibilities, and spectroscopic (IR and far-IR, ligand field, ESR) studies. A variety of stereochemistries is assigned for the complexes in the solid state. The neutral ligand acts as a bidentate chelating agent with ligated atoms being the ring N and the secondary amide O; the LH- ion behaves as a bidentate chelating Nring, Nsecondary amide or as a tridentate Nring, Nsecondary amide, Oprimary amide ligand depending mainly on the reaction conditions.

ΙT 157979-82-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of transition metal complexes)

157979-82-3 CAPLUS RN

2-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME) CN

L70 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:323221 CAPLUS

DOCUMENT NUMBER: 120:323221

TITLE: New molecular frameworks: formation of helical

secondary structures in a group of

oligoanthranilamides

Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew AUTHOR(S):

CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260,

USA

SOURCE: Angewandte Chemie (1994), 106(4), 465-7 (See also

Angew. Chem., Int. Ed. Engl., 1994, 33(4), 446-8)

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE:

Journal

LANGUAGE:

German

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Helical oligoanthranilamide I (R = CO2Me) was prepared from 2,6-pyridinedicarbonyl dichloride and aminobenzamide derivative II (Y = NH2).

II (Y = NH2) prepared from 2-nitrobenzoyl chloride condensation with anthranilic acid Me ester to give II, Y = NO2 followed by catalytic hydrogenation. I (R = CO2Me) was characterized by proton NMR and x-ray crystallog. and the nature of its helical structure discussed. Helical oligoanthranilamide III was also characterized by x-ray crystallog.

IT 155139-01-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure and proton NMR of, conformational anal. in relation to)

RN 155139-01-8 CAPLUS

CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

IT 155138-99-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure of)

RN 155138-99-1 CAPLUS

CN Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

L70 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:162351 CAPLUS

DOCUMENT NUMBER: 96:162351

10/698643

TITLE:

Anthranilic acid derivatives

PATENT ASSIGNEE(S):

Kyoto Pharmaceutical Industries, Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56161362 PRIORITY APPLN. INFO.:	A2	19811211	JP 1980-43744 JP 1980-43744	19800403 19800403

OTHER SOURCE(S):

CASREACT 96:162351

GΙ

- AB Four anthranilic acid derivs. I (R = NO2, NH2, nicotinamido; R1 = Me, H), having smooth muscle-relaxing or contracting activity (no data), were prepared from Me 2-amino-3,4,5-trimethoxybenzoate (II). Thus, 2.45 g II acylated with 1.9 g 2-nitrobenzoyl chloride in CHCl3 gave 82% I (R = NO2, R1 = Me), which was reduced over Pd-C to give I (R = NH2, R1 = Me). Acylation with nicotinoyl chloride gave I (R = nicotinamido, R1 = Me) (III), which was hydrolyzed with 0.5 N NaOH at 40-50° to give I (R = nicotinamido, R1 = H). III was also prepared by cultivating Aspergillus terreus afficanus IFO 8835.
- IT 81469-77-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

- RN 81469-77-4 CAPLUS
- CN Benzoic acid, 3,4,5-trimethoxy-2-[[2-[(3-pyridinylcarbonyl)amino]benzoyl]a mino]-, methyl ester (9CI) (CA INDEX NAME)

Searcher :

Shears

571-272-2528

IT 81469-76-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 81469-76-3 CAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-2-[[2-[(3-pyridinylcarbonyl)amino]benzoyl]a mino]- (9CI) (CA INDEX NAME)

L70 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1980:586283 CAPLUS

DOCUMENT NUMBER:

93:186283

TITLE:

Some reactions of 2-heterocycle-4(3H)-quinazolinones

with electrophilic reagents

AUTHOR(S):

Muraoka, Keiji; Ichikawa, Masataka; Hisano, Takuzo

CORPORATE SOURCE: SOURCE:

Fac. Pharm. Sei., Kumamoto Univ., Japan Yakugaku Zasshi (1980), 100(4), 375-85

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE:

Journal

LANGUAGE:

Japanese

OTHER SOURCE(S):

CASREACT 93:186283

GΙ

AB 2-(1-Oxido-2-pyridino)-3-phenyl-4(3H)-quinazolinone (I), 2-(1-oxido-2-pyridinio)-3-phenyl-4(3H)-quinazolinone 1-oxide, and the control compound, 3-phenyl-2-(2-pyridyl-4(3H)-quinazolinone (II) were nitrated under appropriate conditions to give 3-(3-nitrophenyl)-2-(1-oxido-2-pyridinio)-4(3H)-quinazolinone, 3-(3-nitrophenyl)-2-(1-oxido-2-pyridinio)-4(3H)-quinazolinone 1-oxide, and 3-(3-nitrophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone or the dinitro derivative 6-nitro-3-(3-nitrophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone selectively and in comparatively higher yield. II was halogenated with N-bromosuccinimide or N-chlorosuccinimide by varying reaction temperature and concentration of H2SO4, and by

adding silver sulfate as an activator, to give 3-(3-bromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone and 6-bromo-3-phenyl-2-(2-pyridyl)-4(3H)-quinazolinone or the dihalides 3-(3,4-dibromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone or 6-bromo-3-(3-bromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone, and a further derivative which was presumably a trihalide.

IT 75359-17-0 75359-18-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of)

RN 75359-17-0 CAPLUS

CN 2-Pyridinecarboxamide, N-[2-[(phenylamino)carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 75359-18-1 CAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[(3-nitrophenyl)amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

L70 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:546545 CAPLUS

DOCUMENT NUMBER:

79:146545

TITLE:

2-Pyridyl-4(3H)-quinazolinones

INVENTOR(S):

Hisano, Takuzo; Ichikawa, Masataka; Ide, Hiroyuki; Noda, Kanji; Nakagawa, Akira; Motomura, Toshiharu

Hisamitsu Pharmaceutical Co., Inc.

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 7 pp.

SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
)	-					
JP 48062779	A2	19730901	JP 1971-98092	19711203		
JP 54034749	В4	19791029				
PRIORITY APPLN. INFO.:			JP 1971-98092	19711203		

GI For diagram(s), see printed CA Issue.

AB Quinazolinones (I) were prepared by cyclizing, e.g., 2-nicotinamido-3'-chlorobenzanilide (II). Thus, heating II 18 hr at 200° gave I (R = m-Cl, pyridyl 3-substituted). Similarly, 18 addnl. I were prepared

IT 39122-37-7

RL: RCT (Reactant); RACT (Reactant or reagent) (cyclization of, pyridylquinazolinone from)

RN 39122-37-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(3-chlorophenyl)amino]carbonyl]phenyl]-(9CI) (CA INDEX NAME)

L70 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:58340 CAPLUS

DOCUMENT NUMBER:

78:58340

TITLE:

Syntheses and pharmacological activities of 2-heterocyclic substituted 4(3H)-quinazolinone

derivatives

AUTHOR(S):

SOURCE:

Hisano, Takuzo; Ichikawa, Masataka; Kito, Go; Nishi,

Tomoyuki

CORPORATE SOURCE:

Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan Chemical & Pharmaceutical Bulletin (1972), 20(12),

2575-84

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE: English AB

The preparation of a series of 2-pyridyl-4(3H)-quinazolinones is described. Studies on the structure-activity relationship demonstrated that 2-pyridyl, 3-pyridyl, and 4-pyridyl substitution at 2 position of quinazolinone ring, and o-, m-, and p-substitution of the aromatic ring at 3 position are suitable for manifestation of hypnotic activity. The order of potency of activities produced by the difference in the position of substitution of substituents at 2 and 3 position decreased in the order of 4-pyridyl, o-tolyl > 3-pyridyl, o-tolyl > 2-pyridyl, o-tolyl. The anthranilates of these 4(3H)-quinazolinones were inactive. A maximum hypnotic effect accompanied with other potent pharmacol. properties was observed in 2-(4-pyridyl)-3-o-tolyl-4(3H)-quinazolinone, the potency of which was equal to or stronger than Methaqualone in mice.

IT 39122-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN39122-37-7 CAPLUS

3-Pyridinecarboxamide, N-[2-[[(3-chlorophenyl)amino]carbonyl]phenyl]-CN (CA INDEX NAME)

L70 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1966:403958 CAPLUS

DOCUMENT NUMBER:

65:3958

ORIGINAL REFERENCE NO.: TITLE:

65:699h,700a-f Syntheses and reactions of imidazoles

AUTHOR(S):

Almirante, L.; Mugnaini, A.; Fritz, L. Polo;

Provinciali, E.

CORPORATE SOURCE:

Lab. Bioterapio Milanese Selvi, Milan

Searcher : 571-272-2528 Shears

10/698643

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SOURCE:
                             Bollettino Chimico Farmaceutico (1966), 105(1), 32-44
                             CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE:
                             Journal
LANGUAGE:
                             Italian
OTHER SOURCE(S):
                             CASREACT 65:3958
     2-Aminopyridine (I) (425 g.), and 450 g. BrCH2CH(OMe)2 (II) in 500 ml.
     toluene refluxed 16 hrs. gave 1-(2,2-di-methoxyethyl)-2-aminopyridinium
     bromide, which was made basic in 400 ml. H2O to yield 322 g.
     1-(2,2-dimethoxyethyl)-2-imino-1,2-dihydropyridine (III), b1 108°;
     HCl salt m. 184-5° (EtOH). Similarly was prepared the 4-methyl derivative of III, b2 137%; picrate m. 147-8° (EtOH). III b2.5
     123-6^{\circ}, was also obtained from 19 g. I, 33.8 g. II, and 20.16
     NaHCO3 by boiling 25 hrs. in 40 ml. PhMe. By this method were prepared the
     6-methyl derivative of III, b1.5 120°, 2-imino-1-(2,2-
     dimethoxyethyl)pyrimidine, b2.5 123° [picrate m. 135-6°
      (EtOH)], and 1-(2,2-dimethoxyethyl)-2-imino-1,2-dihydrothiazole, b2
     112°; HCl salt m. 156-7° (iso-PrOH). III (322 g.) was added
     slowly to 1750 ml. H2SO4 at 0° and the solution kept 5 hrs. at
     90° to give 203 g. imidazo[1,2-a]pyridine (IV), b0.5 97°
     [n]20D 1.6211; picrate m. 216-17° (EtOH). Similarly,
     5-methylimidazo[1,2-a]pyridine, b1.5 109° [picrate m. 232-3°
      (EtOH)], 7-methylimidazo[1,2-a]pyridine b0.7 113° [picrate m.
     223-4° (EtOH)], imidazo[1,2-a]pyrimidine, m. 131-3° (C6H6),
     and imidazo[1,2-b]thiazole, b2 106° [picrate m. 205-6°
     (EtOH)], were prepared II (11.2 g.) in 11 ml. H2O containing 2.5 ml. 48%
     shaken 2 hrs., poured into 150 ml. H2O, treated with 25 g. NaHCO3 and 8 g.
     5-bromo-2-aminopyridine, and shaken 7 hrs. at 20° to give 76%
     6-bromoimidazo[1,2-a]pyridine, b1.5 165°, m. 53-5°;
     perchlorate, m. 236-8° (EtOH). Similarly, 6-chloroimidazo[1,2-a]pyridine, b1.5 132° [perchlorate m. 223-4° (EtOH)] was
     prepared 2-Aminopyrimidine (19 g.), and 13.7 g. BrCH2OMe suspended in 80 ml.
     EtOH was heated 3 hrs. at 60^{\circ} to give 29% 2-methylimidazo[1,2-a]pyrimidine hydrobromide, m. 254-5°. Similarly, 2-methylimidazo[1,2-\alpha]pyridine b2 105° [HCl salt,
     195-6° (EtOH)], and 2,5-dimethylimidazo[1,2-\alpha]pyridine b0.5
     112° [perchlorate 215-16° (EtOH)] were obtained. IV (5.9
     g.) and 2.25 g. Me2NH in AcOH was mixed with 1.5 g. HCHO and 25 ml. AcOH, and heated 3 hrs. at 60^{\circ} to give 6.7 g. hygroscopic
     3-(dimethylaminomethyl)imidazo[1,2-\alpha]pyridine, m. 80-1° (ligroine); methiodide m. 233-4° (EtOH). Similarly,
     2-methyl-2-(dimethylaminomethyl)imidazo[1,2-\alpha]pyridine-2HCl, m.
     250-1° (EtOH-Et2O) [methiodide m. 200-1° (decomposition) (EtOH)], 2-methyl-3-(diethylaminomethyl)imidazo[1,2-\alpha]pyridine-2HCl.H2O, m.
     203° (decomposition) (EtOH-Et2O), 2-methyl-3-(morpholinomethyl)imidazo
     [1,2-\alpha]pyridine, m. 93-5° (ligroine), 2-methyl-3-[4(\beta-
     hydroxyethyl)-piperazin-1-ylmethyl]imidazo [1,2-\alpha]pyridine, m.
     167-9° (C6H6C6H12), 2-methyl-3-[bis-(2-
     hydroxyethyl) aminomethyl] imidazo1, 2-α] pyridine, m. 114-16°
     (C6H6), 7-methyl-3-(dimethylaminomethyl)imidazo[1,2-\alpha]pyridine-2HCl,
     250-2° (C6H6) [methiodide m. 232-3° (decomposition) (EtOH)], and
     2-(p-chlorophenyl)-3-(di-methylaminomethyl)imidazo[1,2-\alpha]pyridine-
     2HCl, m. 222-4° (EtOH-Et2O), [methiodide m. 220-22°
     (decomposition) (EtOH)], were prepared IV (11.8 g.) in 20 ml. Me2NCHO was
treated
     with 46.5 g. POCl3 in 60 ml. Me2 NCHO with shaking at 0° and then
```

Searcher: Shears 571-272-2528

to yield the corresponding acyl halide, which without further separation, was

condensed with I or its derivs. Compds. prepared include 4-[p-(nicotinoylamino)benzoyl]aminoantipyrine (III), 55.4%; the p-(nicotinoylamino)benzoyl; p-methylamino analog 93.3%; the 4-N-Me

derivative

of III, the 4-N-benzyl derivative of III, 34.7.%; and 4-N-methyl-4-Nnicotinoylanthranilylaminoantipyrine. Condensation of I with II yielded,

owing to ring closure, $2-(\beta-pyridy1)-3-(4-antipyriny1)-4-quinazolone,$ instead of the expected condensation compound

RN 6188-07-4 CAPLUS

CN Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)- (7CI, 8CI) (CA INDEX NAME)

FILE 'REGISTRY' ENTERED AT 14:48:42 ON 12 NOV 2004

L71 56 SEA FILE=REGISTRY ABB=ON PLU=ON (155138-99-1/BI OR 155139-01-8/BI OR 39122-37-7/BI OR 6188-07-4/BI OR 157864-28-3/BI OR 157979-82-3/BI OR 168284-90-0/BI OR 169043-36-1/BI OR 169043-37 -2/BI OR 169044-06-8/BI OR 169044-07-9/BI OR 169044-08-0/BI OR 169044-09-1/BI OR 169044-10-4/BI OR 169044-11-5/BI OR 169044-56 -8/BI OR 171010-53-0/BI OR 171010-58-5/BI OR 173055-91-9/BI OR 173056-05-8/BI OR 173056-17-2/BI OR 173056-21-8/BI OR 173056-46 -7/BI OR 173056-75-2/BI OR 173056-88-7/BI OR 173056-95-6/BI OR 173056-96-7/BI OR 173056-97-8/BI OR 173057-04-0/BI OR 173057-19 -7/BI OR 173094-25-2/BI OR 180133-05-5/BI OR 180133-06-6/BI OR 192723-63-0/BI OR 196311-73-6/BI OR 196311-77-0/BI OR 196311-92 -9/BI OR 196311-95-2/BI OR 196312-02-4/BI OR 196312-04-6/BI OR 196312-07-9/BI OR 200709-28-0/BI OR 206873-73-6/BI OR 206873-74 -7/BI OR 206873-76-9/BI OR 206873-77-0/BI OR 206873-78-1/BI OR 214203-38-0/BI OR 214203-39-1/BI OR 214203-40-4/BI OR 214203-41 -5/BI OR 216656-75-6/BI OR 75359-17-0/BI OR 75359-18-1/BI OR 81469-76-3/BI OR 81469-77-4/BI)

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=>
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$$G_1$$
 N
 G_1
 N
 G_1
 N

chain nodes :

7 8 10 11 12 14

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21

chain bonds :

5-7 6-11 7-8 8-10 11-12 11-14

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21$

exact/norm bonds :

5-7 7-8 8-10 11-12 11-14

exact bonds :

6-11

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21$

isolated ring systems :

containing 1:

G1:0,S

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS

L6 STRUCTURE UPLOADED

=> dis 16 L6 HAS NO ANSWERS L6 STR

G1 0, S

Structure attributes must be viewed using STN Express query preparation.

 \Rightarrow s 16 sam

SAMPLE SEARCH INITIATED 08:57:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 442 TO ITERATE

100.0% PROCESSED 442 ITERATIONS 24 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS:

7579 TO 10101

PROJECTED ANSWERS:

187 TO

L7

24 SEA SSS SAM L6

=> s 16 full

FULL SEARCH INITIATED 08:57:38 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 8762 TO ITERATE

100.0% PROCESSED 8762 ITERATIONS 569 ANSWERS

SEARCH TIME: 00.00.01

L8569 SEA SSS FUL L6

=> file hcaplus

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SINCE FILE TOTAL ENTRY SESSION 314.03 155.42

FULL ESTIMATED COST

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=> s 18

L9 75 L8

=> s 19 and pd<march 2000 20458207 PD<MARCH 2000 (PD<20000300)

L10 33 L9 AND PD<MARCH 2000

=> dis his

L6 STRUCTURE UPLOADED

L7 24 S L6 SAM L8 569 S L6 FULL

FILE 'HCAPLUS' ENTERED AT 08:57:45 ON 15 NOV 2004

L9 75 S L8

L10 33 S L9 AND PD<MARCH 2000

=> dis 110 1-33 bib abs hitstr

L10 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:880369 HCAPLUS

DN 135:40545

TI Phase I trial of XR9576 in healthy volunteers demonstrates modulation of P-glycoprotein in CD56+ lymphocytes after oral and intravenous administration

AU Stewart, Alistair; Steiner, Jan; Mellows, Graham; Laguda, Bim; Norris, David; Bevan, Paul

CS Xenova, Ltd., Slough, SL1 4EF, UK

SO Clinical Cancer Research (2000), 6(11), 4186-4191 CODEN: CCREF4; ISSN: 1078-0432

PB American Association for Cancer Research

DT Journal

LA English

- XR9576 is a novel inhibitor of P-glycoprotein (P-gp) that has been shown AB to reverse P-gp-dependent multidrug-resistance in tumor cell lines and tumor-bearing animals. This work reports the i.v. and oral administration of XR9576 to healthy volunteers in dose-escalating studies with the aim of investigating its safety, its pharmacokinetics, and effects on a surrogate marker of efficacy (CD56+ lymphocytes instead of tumors). XR9576 was administered as a single dose-upward titration of 0.1, 0.2, 0.5, 1.0, and 2 mg/kg i.v. or 50, 100, 200, 500, and 750 mg/volunteer orally. surrogate marker for in vivo efficacy examined the accumulation of the P-gp substrate Rhodamine-123 (Rh-123) in P-gp-expressing CD56+ lymphocytes by flow cytometry. Addition of Rh-123 to blood from subjects given XR9576 or a placebo demonstrated drug-dependent modulation of P-gp activity. the lowest doses, significant effects on Rh-123 accumulation in CD56+ cells were observed Maximal effects occurred during the i.v. infusion or 4-6 h after oral administration. As the dose was increased, a concomitant rise in the extent and duration of P-gp blockade was observed A dose of 2.0 mg/kg i.v. and ≥ 200 mg/volunteer orally gave .apprx.100% inhibition of P-qp for >24 h. All doses of XR9576 tested were well tolerated. Inhibition increased with plasma XR9576 concentration, and maximal activity was achieved at 150-200 ng XR9576/mL. In conclusion, XR9576 produced sustained inhibition of P-gp after i.v. and oral administration. Supported by the elimination half-life of about 24 h, XR9576 is being taken into Phase II trials as a once-daily agent.
- IT **206873-63-4,** XR 9576

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(XR9576 modulation of P-glycoprotein in CD56+ lymphocytes after oral and i.v. administration to humans)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:695199 HCAPLUS

DN 134:5213

TI Folding Dendrons: The Development of Solvent-, Temperature-, and Generation-Dependent Chiral Conformational Order in Intramolecularly Hydrogen-Bonded Dendrons

AU Recker, Janosch; Tomcik, Dennis J.; Parquette, Jon R.

CS Department of Chemistry, The Ohio State University, Columbus, OH, 43210,

SO Journal of the American Chemical Society (2000), 122(42), 10298-10307 CODEN: JACSAT; ISSN: 0002-7863

American Chemical Society

DT Journal

PB

LA English

AB The synthesis of intramolecularly hydrogen-bonded dendrons with stereogenic terminal groups derived from (1S,2S)-(+)-thiomicamine up to the third generation is described. CD studies reveal that the equilibrium interconverting two diastereomeric helical conformations (M and P helixes) relating a pair of anthranilamide termini depends on solvent, temperature, and dendrimer generation. A conformational preference for M-type helicity along the periphery of the dendrons increased with increasing dendrimer generation and in poor solvents as observed by CD. Equilibration of these diastereomeric helical conformations is rapid at the first generation in all solvents and at all temps. investigated; however, at the second generation the equilibrium begins to bias a single diastereomeric helical conformation along the periphery that becomes maximal at low temps. and in poor solvents. At the third generation, the helical bias is intrinsically higher so that the conformational preference of the termini becomes much less sensitive to solvent and temperature, and the unfolding process becomes more difficult. We propose that nonbonded repulsive interactions that increase with generation and in poor solvents couple the motions and conformational preferences of each pair of terminal groups through their correlated rotations and contribute to the stability of the M helical conformation of the terminal groups. This represents the first example of well-defined asym. secondary structure occurring in a dendrimer system.

IT 308245-27-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(in preparation and characterization of intramolecularly hydrogen-bonded dendrimer)

RN 308245-27-4 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[[(1S,2S)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-[4-(methylthio)phenyl]ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 308245-25-2P 308245-26-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

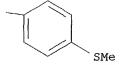
(in preparation and characterization of intramolecularly hydrogen-bonded dendrimer)

RN 308245-25-2 HCAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[[[(1S,2S)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-[4-(methylthio)phenyl]ethyl]amino]carbonyl]phenyl]-4-chloro-(9CI) (CA INDEX NAME)

RN

2,6-Pyridinedicarboxamide, N,N'-bis[2-[[[(1S,2S)-2-(acetyloxy)-1-[(acetyloxy)methyl]-2-[4-(methylthio)phenyl]ethyl]amino]carbonyl]phenyl]-4-amino- (9CI) (CA INDEX NAME) CN



RE.CNT 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

2000:621133 HCAPLUS AN

DN 133:305245

ΤI Drug Binding Sites on P-Glycoprotein Are Altered by ATP Binding Prior to Nucleotide Hydrolysis

ΑU Martin, Catherine; Berridge, Georgina; Mistry, Prakash; Higgins, Christopher; Charlton, Peter; Callaghan, Richard

Nuffield Department of Clinical Laboratory Sciences John Radcliffe CS

Hospital, University of Oxford, Oxford, OX3 9DU, UK Biochemistry (2000), 39(39), 11901-11906 CODEN: BICHAW; ISSN: 0006-2960 SO

PB American Chemical Society

DTJournal

LА English

AΒ P-qlycoprotein (P-qp) confers multiple drug resistance on cancer cells by acting as a plasma membrane localized ATP-dependent drug efflux pump. Currently, there is little information on the nature of the communication between the energy-providing nucleotide binding domains (NBDs) and the drug binding sites of P-gp to generate transport of substrate. Many substrates and modulators cause alterations in ATP hydrolysis, but what effect do the various stages of the catalytic cycle have on drug interaction with P-gp. Vanadate trapping of Mg·ADP caused a reversible decrease in the binding capacity of the transported substrate [3H]-vinblastine and the nontransported modulator [3H]XR9576 to P-gp in CHrB30 cell membranes. The non-hydrolyzable nucleotide analog ATP- γ -S also caused a reduction in the binding capacity of [3H]-vinblastine but not for the modulator [3H]XR9576. This indicates that signaling to the NBDs following binding of a nontransported modulator is different to that transmitted upon interaction of a transported substrate. Second, it appears that the binding of nucleotide, rather than its hydrolysis, causes the initial conformational shift in the drug-binding site during a transport cycle.

IT 206873-63-4, XR 9576

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(XR 9576; drug binding sites on P-glycoprotein are altered by ATP

binding prior to nucleotide hydrolysis in relation to multiple drug resistance rit conformational shift)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

MeO
$$N - CH_2 - CH_2$$
 $MeO - NH - C$ $NH - C$ $NH - C$ $MeO - NH - C$ $MeO - NH - C$

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:614974 HCAPLUS

DN 133:291075

TI Communication between multiple drug binding sites on P-glycoprotein

AU Martin, Catherine; Berridge, Georgina; Higgins, Christopher F.; Mistry, Prakash; Charlton, Peter; Callaghan, Richard

CS Department of Clinical Laboratory Sciences, John Radcliffe Hospital, University of Oxford, UK

SO Molecular Pharmacology (2000), 58(3), 624-632 CODEN: MOPMA3; ISSN: 0026-895X

PB American Society for Pharmacology and Experimental Therapeutics

DT Journal

LA English

AB

P-qlycoprotein, a member of the ATP-binding cassette transporter family, is able to confer resistance on tumors against a large number of functionally and chemical distinct cytotoxic compds. Several recent investigations suggest that P-glycoprotein contains multiple drug binding sites rather than a single site of broad substrate specificity. In the present study, radioligand-binding techniques were used to directly characterize drug interaction sites on P-glycoprotein and how these multiple sites interact. The drugs used were classified as either (1) substrates, which are known to be transported by P-glycoprotein (e.g., vinblastine) or (2) modulators, which alter P-glycoprotein function but are not themselves transported by the protein (e.g., XR9576). Drug interactions with P-glycoprotein were either competitive, at a common site, or noncompetitive, and therefore at distinct sites. Based on these data, we can assign a min. of four drug binding sites on P-glycoprotein. These sites fall into two categories: transport, at which translocation of drug across the membrane can occur, and regulatory sites, which modify P-glycoprotein function. Intriguingly, however, some modulators interact with P-glycoprotein at a transport site rather than a regulatory site. The pharmacol. data also demonstrate that both transport and regulatory sites are able to switch between high- and low-affinity conformations. The multiple sites on P-glycoprotein display complex allosteric interactions through which interaction of drug at one site switches other sites between high- or low-affinity conformations. The data are discussed in terms of a model for the mechanism of transport

by P-glycoprotein.

IT 206873-63-4, XR 9576

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(communication between multiple drug binding sites on P-glycoprotein)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

MeO
$$N$$
 CH_2 CH_2 MeO NH C NH C NH C NH C NH C MeO

RE:CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:68948 HCAPLUS

DN 132:251284

TI Total Synthesis of the Fumiquinazoline Alkaloids: Solution-Phase Studies

AU Wang, Haishan; Ganesan, A.

CS Institute of Molecular and Cell Biology, National University of Singapore, Singapore, 117609, Singapore

SO Journal of Organic Chemistry (2000), 65(4), 1022-1030 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

Ι

DT Journal

LA English

OS CASREACT 132:251284

GI

II

AB Biomimetic total syntheses of glyantrypine (I), fumiquinazoline F, fumiquinazoline G, and fiscalin B were achieved in four steps from

tryptophan Me ester. In the key step, the anthranilamide residue in a linear tripeptide is dehydrated to a benzoxazine, e.g. II, by reaction with triphenylphosphine, iodine, and a tertiary amine. The benzoxazines subsequently undergo rearrangement to the natural products via an amidine intermediate. This dehydrative oxazine to quinazoline route is applicable to a broad range of N-acylanthranilamides, including sterically hindered cases.

IT 262590-33-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(total synthesis of fumiquinazoline alkaloids, solution-phase studies)
262590-33-0 HCAPLUS

RN 262590-33-0 HCAPLUS
CN 2-Quinolinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:651313 HCAPLUS

DN 132:8771

TI The molecular interaction of the high affinity reversal agent XR9576 with P-glycoprotein

AU Martin, Catherine; Berridge, Georgina; Mistry, Prakash; Higgins, Christopher; Charlton, Peter; Callaghan, Richard

CS Nuffield Department of Clinical Biochemistry & Cellular Science, John Radcliffe Hospital, University of Oxford, Oxford, OX3 9DU, UK

SO British Journal of Pharmacology (1999), 128(2), 403-411 CODEN: BJPCBM; ISSN: 0007-1188

PB Stockton Press

DT Journal

LA English

1 The kinetics and nature of equilibrium binding were used to characterize the ΑB mol. interaction of the anthranilic acid derivative [3H]-XR9576 with the multidrug resistance P-glycoprotein (P-gp). XR9576 displayed specific high-affinity binding to P-gp (Bmax = 275 pmol mg-1, Kd=5.1 nM). The transport substrates [3H]-vinblastine and [3H]-paclitaxel displayed 4 fold and 20 fold lower affinity resp. for P-gp. The duration of action of XR9576 with P-gp was increased in comparison to that of vinblastine which displayed a slower rate of association and a faster dissociation rate. 2 The relative affinities of several modulators and transport substrates to interact with P-gp were determined from displacement drug equilibrium binding assays. Vinblastine and paclitaxel could only fractionally displace [3H]-XR9576 binding, displaying Ki values significantly different from their measured Kd values. This suggests a non-competitive interaction between XR9576 and the P-gp substrates vinblastine and paclitaxel. 3 XR9576 was shown to be a potent modulator of P-gp mediated [3H]-vinblastine and [3H]-paclitaxel transport as it increased the steady-state accumulation of these cytotoxics in CHrB30 cells to levels

observed in non-P-gp-expressing AuxB1 cells (EC50 = 487 ± 50 nM). This inhibition of drug transport is not mediated through competition for transport since [3H]-XR9576 accumulation was not influenced by P-gp expression or function. 4 These results demonstrate that the P-gp modulator XR9576 exhibits greater selectivity, duration of inhibition and potency of interaction with this transporter than any other reported modulators. Several lines of evidence suggest that XR9576 inhibits P-gp function by binding at a site which is distinct from the site of interaction of transport substrates. The two sites may be classified as serving modulatory or transport functions.

IT 206873-63-4, XR 9576

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(mol. interaction of high affinity reversal agent XR9576 with P-qlycoprotein)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

MeO
$$N-CH_2-CH_2$$
 MeO $N+C$ $N+C$

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:188605 HCAPLUS

DN 131:340

TI Reversal of P-glycoprotein mediated multidrug resistance by novel anthranilamide derivatives

AU Roe, Michael; Folkes, Adrian; Ashworth, Philip; Brumwell, Julie; Chima, Lal; Hunjan, Sukhjit; Pretswell, Ian; Dangerfield, Wendy; Ryder, Hamish; Charlton, Peter

CS Xenova Ltd., Slough, SL1 4EF, UK

SO Bioorganic & Medicinal Chemistry Letters (1999), 9(4), 595-600 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB We have synthesized and evaluated a series of anthranilamide based modulators of P-glycoprotein. These studies have identified XR9576, a potent inhibitor of P-glycoprotein in vitro and in vivo. The general synthesis and the SAR of these compds. are described.

IT 206872-35-7P 206873-60-1P 206873-61-2P 206873-62-3P 206873-63-4P 206873-65-6P 206873-66-7P 206873-68-9P 206873-69-0P 206873-71-4P 206873-73-6P 206873-74-7P

206873-78-1P 225938-12-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel anthranilamide derivs. for reversal of P-glycoprotein mediated multidrug resistance)

RN 206872-35-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny1)ethy1]phenyl]amino]carbonyl]-4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{MeO} & & & \\ & & & \\ \text{MeO} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

RN 206873-60-1 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny1)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-61-2 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(lH)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-5-fluorophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ \text{MeO} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN · 206873-62-3 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-fluorophenyl]- (9CI) (CA INDEX NAME)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

MeO
$$N-CH_2-CH_2$$
 MeO $NH-C$ $NH-C$

RN 206873-65-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny1)ethy1]pheny1]amino]carbony1]-5-nitropheny1]- (9CI) (CA INDEX NAME)

RN 206873-66-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-methylphenyl]- (9CI) (CA INDEX NAME)

RN 206873-68-9 HCAPLUS

CN 3-Quinolinecarboxamide, N-[4-chloro-2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-69-0 HCAPLUS

CN 3-Quinolinecarboxamide, N-[5-chloro-2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ \text{MeO} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 206873-71-4 HCAPLUS

CN 2-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ &$$

RN 206873-73-6 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{MeO} \end{array}$$

RN 206873-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 206873-78-1 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-6-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 225938-12-5 HCAPLUS

CN 3-Isoquinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT '

L10 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:42569 HCAPLUS

DN 130:95392

TI Preparation of bis-amides of 1,2-benzenediamines as antithrombotic agents

Beight, Douglas Wade; Craft, Trelia Joyce; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Klimkowski, Valentine Joseph; Kyle, Jeffrey Alan; Masters, John Joseph; Mendel, David; Milot, Guy; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

PA Eli Lilly and Company, USA

SO PCT Int. Appl., 311 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 9900121 A1 19990107 WO 1998-US13427 19980626 <-
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,

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DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG,
             KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
             NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
             UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, ML, MR, NE, SN, TD, TG
     AU 9882708
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                                 19990119
                                             AU 1998-82708
                                                                     19980626 <--
     EP 1014962
                           A1
                                 20000705,
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                                                                     19980626
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
     JP 2002512633
                           T2
                                 20020423
                                             JP 1999~505829
                                                                     19980626
                           В1
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                                             US 2000-445972
                                                                     20000320
     US 6313122
     US 2002120007
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                                             US 2001-961164
                                                                     20010921
     US 6605626
                           B2
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PRAI US 1997-50894P
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                                 19970626
     WO 1998-US13427
                                 19980626
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                           АЗ
                                 20000320
     US 2000-445972
os
     MARPAT 130:95392
GΙ
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The title compds. [I; A3-A6 together with the two carbons to which they are attached = (un)substituted benzene wherein A3 = CR3; A4 = CR4; A5 = CR5; A6 = CR6; R3 = H, OH, OCH2Ph, etc.; R4, R5 = H, Me, halo, etc.; R6 = H, F, OH, etc.; two adjacent residues selected from R3-R6 together form a benzene ring, and the other two are hydrogen; L1 = NHCO, OCO, CONH; Q1 = (un)substituted Ph, 2-furanyl, 2-thienyl, etc.; R2 = (un)substituted NHCOPh, OCOPh, CH2OPh, etc.], useful as inhibitors of factor Xa (no data), were prepared and formulated. Thus, treatment of N-benzylisonipecotate with oxalyl chloride in CH2Cl2 followed by addition of DMF, and subsequent addition of the resulting mixture into a solution of N1-(4-methoxybenzoyl)-1,2-benzenediamine and pyridine in CH2Cl2 and THF afforded 54% II. Compds. I are effective at 0.01-1000 mg/kg/day.

IT 219492-67-8P 219492-69-0P 219492-71-4P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bis-amides of 1,2-benzenediamines as antithrombotic agents) 219492-67-8 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(4-chlorophenyl)amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

RN 219492-69-0 HCAPLUS

CN Pyridinium, 4-[[[2-[[(4-chlorophenyl)amino]carbonyl]phenyl]amino]carbonyl]1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 219492-71-4 HCAPLUS

CN Pyridinium, 4-[[[2-[[(4-chlorophenyl)amino]carbonyl]phenyl]amino]carbonyl]1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)

• Br

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:724208 HCAPLUS

DN 130:33033

Chromium picolinate complexes and pharmaceuticals with hypoglycemic or TΙ insulin-lowering effect

Kuroki, Yasuhisa IN

Otsuka Pharmaceutical Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 8 pp. SO

CODEN: JKXXAF

DΤ Patent

LΑ Japanese

GΙ

FAN.CN'	T 1 ATENT NO.	KIND	DATE	APPLICATION NO.	 DATE	
PRAI J	P 10298189 P 1997-112682 ARPAT 130:33033	A2	19981110 19970430	JP 1997-112682	19970430 <	<

Hypoglycemic agents, their compns., or insulin-lowering compns. contain Cr AΒ complexes I [R1-R3 = H, lower alkyl, OH, benzoyl, lower alkoxycarbonyl, halo-substituted 3-(lower alkyl)-4(3H)-quinazolin-2-yl; R1 = R2 = R3≠ H] and optional carriers. 3-Hydroxypicolinic acid (4.17 g) was treated with 2.66 g CrCl3.6H2O in H2O at 80° for 5 h to give 1.67 g trans-I.1/2H2O (R1 = OH, R2 = R3 = H), which was orally administered to dexamethasone-treated rats to show 5% decrease of blood glucose (at 10 mg/kg dose) and 25% decrease of blood insulin (at 100 mg/kg dose). Formulation examples are given.

 \mathbf{IT} 216656-75-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chromium picolinate complexes as hypoglycemic or insulin-lowering agents)

216656-75-6 HCAPLUS RN

2-Pyridinecarboxylic acid, 5-[[[5-chloro-2-[(methylamino)carbonyl]phenyl]a CN mino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ MeO-C & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

L10 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:606819 HCAPLUS

DN 129:297543

TI Synthesis and structure of chiral 2,6-bis[(2-carbamoylphenyl)carbamoyl]pyr idine ligands

AU Yu, Qiang; Baroni, Timothy E.; Liable-Sands, Louise; Rheingold, Arnold L.; Borovik, A. S.

CS Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA

SO Tetrahedron Letters (1998), 39(38), 6831-6834 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

The synthesis and structure of enantiomerically pure 2,6-bis[(2-carbamoylphenyl)carbamoyl]pyridine ligands are described. Appended from the aryl groups are optically active groups which provide a chiral environment around the planar pyridine core. NMR and x-ray diffraction studies show that these ligands contain helical character which is maintained by a network of intramol. H bonds. These ligands can bind metal ions through their tridentate diamidato-pyridyl chelate to form optically active metal complexes. A Ni complex is prepared and its x-ray crystal structure is determined The modular design of these ligands offers a variety of chiral environments about the metal chelate that can be useful in the synthesis of metal reagents for asym. transformations.

IT 214203-39-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with nickel)

RN 214203-39-1 HCAPLUS

CN L-Valine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

IT 214203-41-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 214203-41-5 HCAPLUS

CN L-Alanine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonyl)]bis-, dimethyl ester, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 214203-38-0 CMF C29 H29 N5 O8

2 CM

CRN 75-09-2 CMF C H2 Cl2

 $_{\text{Cl}-\text{CH}_2-\text{Cl}}$

214203-38-0P IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)

214203-38-0 HCAPLUS RN

L-Alanine, N,N'-[2,6-pyridinediylbis(carbonylimino-2,1-CN phenylenecarbonyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 214203-40-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

214203-40-4 HCAPLUS RN

2,6-Pyridinedicarboxamide, N,N'-bis[2-[[[(1S)-1-CNphenylethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 21 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN L10

ΑN 1998:351844 HCAPLUS

DN 129:40989

Preparation of N-(2-oxoethyl)benzamides as cysteine protease inhibitors ΤI

IN Lubisch, Wilfried; Moeller, Achim; Treiber, Hans-Joerg

PA

BASF A.-G., Germany Ger. Offen., 34 pp. SO

CODEN: GWXXBX

DTPatent

LА German

FAN.	CNT 1							
		T NO.					APPLICATION NO.	DATE
ΡΙ	DE 19 CA 22 WO 98	648793 72388 23581 : AL,	AU,	BG,	A1 AA A1 BR,	19980528 19980604 19980604 BY, CA, CN,	DE 1996-19648793 CA 1997-2272388 WO 1997-EP6292 CZ, GE, HU, ID, IL,	19971111 < 19971111 < JP, KR, KZ, LT,
		•	•		•		SG, SI, SK, TR, UA,	US, AM, AZ, BY,
	AU 98	W: AT, 54814	BE,	CH,	DE, Al	19980622	FR, GB, GR, IE, IT, AU 1998-54814	
						20011220		10071171
						,	EP 1997-951172	
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	CN 12	38761 [°]	·		Α	19991215	CN 1997-180091	19971111 <
	BR 97	13147			Α	20000208	BR 1997-13147	19971111 <
	NZ 33	5542			Α	20000728	NZ 1997-335542	19971111
	JP 20	015065	96		Т2	20010522	JP 1998-524208	19971111
	RU 21	89973			C2	20020927	RU 1999-113461	19971111
	ZA 97	10569			Α	19990525		
	TW 39	3454			В	20000611		
		02492			Α	19990525		
		000572	27	•		20000915		
	US 62	51917			B1.	20010626	US 1999-297916	19990526

PRAI DE 1996-19648793 A 19961126 WO 1997-EP6292 W 19971111

OS MARPAT 129:40989

AB R1Z1Z2CONHCHR3CHO [R1 = (un)substituted (hetero)aryl; R3 = [(hetero)aryl] hydrocarbyl; Z1 = bond, O, CO, alkylene, etc.; Z2 = (un)substituted phenylene] were prepared Thus, 2-PhC6H4CO2H was amidated by (S)-PhCH2CH(NH2)CH2OH and the product oxidized to give (S)-2-PhC6H4CONHCH(CH2Ph)CHO (I). Data for biol. activity of I were given.

IT 208174-55-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-(2-oxoethyl) benzamides as cysteine protease inhibitors)

RN 208174-55-4 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[(15)-1-formyl-2-phenylethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 208175-35-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of N-(2-oxoethyl)benzamides as cysteine protease inhibitors)

RN 208175-35-3 HCAPLUS CN 3-Pyridinecarboxamide, N-[2-[[[(1S)-1-(hydroxymethyl)-2-

phenylethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:268489 HCAPLUS

DN 128:321568

- TI Anthranilic acid derivatives as multi drug resistance modulators
- IN Ryder, Hamish; Ashworth, Philip Anthony; Roe, Michael John; Brumwell, Julie Elizabeth; Hunjan, Sukhjit; Folkes, Adrian John; Sanderson, Jason Terry; Williams, Susannah; Maximen, Levi Michael; et al.
- PA Xenova Ltd., UK; Ryder, Hamish; Ashworth, Philip Anthony; Roe, Michael John; Brumwell, Julie Elizabeth; Hunjan, Sukhjit; Folkes, Adrian John; Sanderson, Jason Terry; Williams, Susannah; Maximen, Levi Michael
- SO PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FAN.	PATENT NO.					KIND DATE				APPLICATION NO.						DATE				
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^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Anthranilic acid derivs. I [R, R1, R2 = H, alkyl, OH, alkoxy, halo, NO2, amino; or R1R2 = OCH2O or OCH2CH2O; R3 = H, alkyl; R4 = alkyl, or CH2 or

CH2CH2 bridged to either Ph ring; R5 = H, OH, alkyl; X = bond, O, S, S(CH2)p, O(CH2)p; p = 1-6; R6 = H, alkyl, alkoxy; q = 0 or 1; Ar = (un)saturated carbo- or heterocyclic; R7, R8 = H, (un)substituted alkyl, alkoxy, OH, halo, Ph, NHOH, NO2, amino, SH, alkylthio; or R7R8 = CH:CHCH:CH or OCH2O; n = 0, 1; m = 0-6] and their pharmaceutically acceptable salts are disclosed. The compds. are inhibitors of P-glycoprotein, and may thus be used, inter alia, as modulators of multidrug resistance in the treatment of multidrug-resistant cancers, for example, to potentiate the cytotoxicity of a cancer drug. For instance, amidation of 3-quinolinecarboxylic acid with the corresponding aminothiophene derivative via the acid chloride gave title compound II in 44% yield. In a test for potentiation of doxorubicin toxicity to AR 1.0 cells, II had a potentiation index of 142 at 30 nM.

IT 206872-32-4P 206872-33-5P 206872-35-7P 206872-40-4P 206872-44-8P 206872-46-0P 206872-49-3P 206872-51-7P 206872-52-8P 206872-53-9P 206872-54-0P 206872-55-1P 206872-56-2P 206872-57-3P 206872-59-5P 206872-60-8P 206872-62-0P 206872-64-2P 206872-65-3P 206872-66-4P 206872-67-5P 206872-68-6P 206872-69-7P 206872-70-0P 206872-71-1P 206872-72-2P 206872-73-3P 206872-74-4P 206872-75-5P 206872-76-6P 206872-78-8P 206872-79-9P 206872-80-2P 206872-84-6P 206872-85-7P 206872-86-8P 206872-87-9P 206872-88-0P 206872-90-4P 206872-91-5P 206872-92-6P 206872-93-7P 206873-39-4P 206873-40-7P 206873-41-8P 206873-44-1P 206873-45-2P 206873-46-3P 206873-47-4P 206873-60-1P 206873-61-2P 206873-62-3P 206873-63-4P 206873-65-6P 206873-66-7P 206873-67-8P 206873-68-9P 206873-69-0P 206873-70-3P 206873-71-4P 206873-72-5P 206873-73-6P 206873-74-7P 206873-75-8P 206873-78-1P 206873-79-2P 206874-31-9P 206874-33-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilic acid derivs. as $\operatorname{multi-drug}$ resistance $\operatorname{modulators}$)

RN 206872-32-4 HCAPLUS

CN 3-Quinolinecarboxamide, 2-chloro-N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-33-5 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-4-hydroxy-7-(trifluoromethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

MeO
$$N - CH_2 - CH_2$$
 $NH - C$ $NH - C$ O OH

PAGE 1-B

__ CF3

RN 206872-35-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 206872-40-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-4-hydroxy- (9CI) (CA INDEX NAME)

206872-44-8 HCAPLUS RN

3-Quinoline carboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]methylamber]]CN mino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2-N-CH_2-CH_2$$
 NH O O C C NH

206872-46-0 HCAPLUS $RN \cdot$

3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-4]]]]]CN isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

MeO
$$N - CH_2 - CH_2$$
 $N - CH_2 - CH_2$ $N - CH_2$

206872-49-3 HCAPLUS RN

3-Quinolinecarboxamide, N-[2-[[4-[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-4]]]]CNisoquinolinyl)ethyl]thio]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-51-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny])ethoxy]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-52-8 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-1-methyl-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-53-9 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(1,3-dihydro-2H-isoindol-2-yl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-54-0 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(6,7-dichloro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 206872-55-1 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(7,8-dichloro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & O \\ C & \\ NH & O \\ C & \\ C &$$

RN 206872-56-2 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl]-(9CI) (CA INDEX NAME)

206872-57-3 HCAPLUS RN

3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethylphenyl)methyl]methylam CN ino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

206872-59-5 HCAPLUS

RN3-Quinolinecarboxamide, N-[2-[[[3-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-1]]]] CN isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

206872-60-8 HCAPLUS RN

3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-7-nitro-2(1H)-CN isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-62-0 HCAPLUS
CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]ethylam ino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2-N-CH_2-CH_2$$
 NH O OMe N O C C

RN 206872-66-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[butyl[(3,4-dimethoxyphenyl)methyl]amino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2-N-CH_2-CH_2$$
 NH O O C NH

RN 206872-67-5 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(4-butoxy-3-methoxyphenyl]methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

RN 206872-68-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-difluorophenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-69-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & Me \\
 & NH-C \\
 & NH-C
\end{array}$$

RN 206872-70-0 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[[3-methoxy-4-(1-methylethoxy)phenyl]methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

i-Pro
$$\begin{array}{c|c} CH_2-N-CH_2-CH_2 \\ \hline Me \\ OMe \\ \hline \\ C-NH \\ \hline \end{array}$$

RN 206872-71-1 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3-hydroxy-4-methoxyphenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

MeO
$$CH_2-N-CH_2-CH_2$$
 NH O O C C

RN 206872-72-2 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[3-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny1)-2-hydroxypropoxy]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & O \\ \hline \\ NH & O \\ \hline \\ C-NH & OH \\ \hline \\ O-CH_2-CH-CH_2-N & OMe \\ \hline \\ OMe \\ \end{array}$$

RN 206872-73-3 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(4-hydroxy-3-methoxyphenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

RN 206872-74-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinoliny1)ethy1]-2-methylphenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-75-5 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]-2-methoxyphenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-76-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[[[[4-methoxy-3-(1-methylethoxy)phenyl]methyl]methylamino]methyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-78-8 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)-1-methylethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

206872-79-9 HCAPLUS RN

3-Quinolinecarboxamide, N-[2-[[[4-[2-[[[4-(dimethylamino)phenyl]methyl]met CNhylamino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-N-CH_2-CH_2 \\ \hline \\ Me \\ \hline \\ N \\ O \\ \hline \\ C-NH \\ \hline \end{array}$$

206872-80-2 HCAPLUS RN

3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3-butoxy-4-CN methoxyphenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]-4,5dimethoxyphenyl] - (9CI) (CA INDEX NAME)

206872-84-6 HCAPLUS

RN3-Quinolinecarboxamide, N-[2-[[[3-[3-(3,4-dihydro-6,7-dimethoxy-2(1H)-CN isoquinolinyl)propyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-85-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[[[[4-methoxy-3-(1-methylethoxy)phenyl]methyl]methylamino]methyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-86-8 HCAPLUS

CN 3-Quinolinecarboxamide, N-[5-chloro-2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 206872-87-9 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(7,8-dihydro-1,3-dioxolo[4,5-g]isoquinolin-6(5H)-yl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 206872-88-0 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(6,7-diethoxy-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206872-90-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]methylamino]ethyl]phenyl]amino]carbonyl]-4,5-difluorophenyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2-N-CH_2-CH_2$$
 NH NH O O C C C

RN 206872-91-5 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]methyla mino]ethyl]phenyl]amino]carbonyl]-5-methylphenyl]- (9CI) (CA INDEX NAME)

RN 206872-92-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl](1-methylethyl)amino]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

MeO
$$i-Pr$$
 OMe $i-Pr$ OMe OMe

RN 206872-93-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[(3,4-dimethoxyphenyl)methyl]methyla mino]ethyl]phenyl]amino]carbonyl]-5-nitrophenyl]- (9CI) (CA INDEX NAME)

RN 206873-39-4 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & & & & \\ \text{MeO} & & & & \\ \text{MeO} & & & & \\ \text{N} & & & & \\ \end{array}$$

RN 206873-40-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-41-8 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-44-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & N \\ NH-C=O \\ & C-NH-CH_2-CH_2-N \\ & O \\ \end{array}$$

RN 206873-45-2 HCAPLUS

CN 2-Quinolinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \hline \\ C - NH - CH_2 - CH_2 - N \end{array}$$
 OMe

RN 206873-46-3 HCAPLUS

CN 3-Isoquinolinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \hline C - NH - CH_2 - CH_2 - N \\ \hline NH & O \\ \hline O & N \\ \hline \end{array}$$

RN 206873-47-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \hline C - NH - CH_2 - CH_2 - N \\ \hline NH & O \\ \hline C & NH \\ \hline O & NH$$

RN 206873-60-1 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-61-2 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-5-fluorophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 206873-62-3 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-fluorophenyl]- (9CI) (CA INDEX NAME)

RN 206873-63-4 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4,5-dimethoxyphenyl]- (9CI) (CA INDEX NAME)

MeO
$$N - CH_2 - CH_2$$
 $N - CH_2 - CH_2$
 $N - CH_2$
 N

RN 206873-65-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-5-nitrophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{MeO} & & & \\ & & & \\ & & & \\ \text{MeO} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 206873-66-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-4-methylphenyl]- (9CI) (CA INDEX NAME)

RN 206873-67-8 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]-5-methylphenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 206873-68-9 HCAPLUS

CN 3-Quinolinecarboxamide, N-[4-chloro-2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-69-0 HCAPLUS

CN 3-Quinolinecarboxamide, N-[5-chloro-2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-70-3 HCAPLUS

CN 3-Quinolinecarboxamide, N-[5-amino-2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 206873-71-4 HCAPLUS

CN 2-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-72-5 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-5,6,7,8-tetrahydro-(9CI) (CA INDEX NAME)

RN 206873-73-6 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206873-74-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} N \\ C = C \\ NH \\ C = C \\$$

RN 206873-75-8 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} N \\ C \\ C \\ O \\ NH \\ CH_2-CH_2 \\ \end{array}$$

RN 206873-78-1 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-6-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{C} \\ \text{C} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{N} \\ \text{C} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text$$

RN 206873-79-2 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-6-methoxy- (9CI) (CA INDEX NAME)

RN 206874-31-9 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-(3,4-dihydro-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$N-CH_2-CH_2$$
 $N+C$
 $N+C$
 $N+C$
 $N+C$

RN 206874-33-1 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)methyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

IT 206874-69-3P 206874-70-6P 206874-71-7P 206874-85-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of anthranilic acid derivs. as multi-drug resistance modulators)

RN 206874-69-3 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-[2-[[dimethyl(1,1,2-trimethylpropyl)silyl]oxy]ethyl]phenyl]amino]carbonyl]phenyl]- (9CI) (CAINDEX NAME)

RN 206874-70-6 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-(2-hydroxyethyl)phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 206874-71-7 HCAPLUS

CN 3-Quinolinecarboxamide, N-[2-[[[4-(2-bromoethyl)phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

206874-85-3 HCAPLUS

Carbamic acid, [4-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-CN isoquinolinyl)ethyl]phenyl]amino]carbonyl]-3-[(3quinolinylcarbonyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) INDEX NAME)

RE.CNT THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN L10

AN 1998:13933 HCAPLUS

DN 128:75193

ΤI Preparation of aminophthalic acid derivatives as pesticides.

Elbe, Hans-Ludwig; Dutzmann, Stefan; Stenzel, Klaus IN

PA Bayer Aktiengesellschaft, Germany

SO PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DTPatent

LΑ German

FAN.	CNT 1					
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE		
PI	WO 9747589	Al 19971218	WO 1997-EP2845	19970602 <		
	W: AU, BB, BG,	BR, BY, CA, CN,	CZ, HU, IL, JP, KR, KZ,	LK, MX, NO,		
	NZ, PL, RO,	RU, SK, TR, UA,	US			
	RW: AT, BE, CH,	DE, DK, ES, FI,	FR, GB, GR, IE, IT, LU,	MC, NL, PT,		
	SE, BF, BJ,	CF, CG, CI, CM,	GA, GN, ML, MR, NE, SN,	TD, TG		
	DE 19623744	A1 19971218	DE 1996-19623744	19960614 <		
	AU 9730936	A1 19980107	AU 1997-30936	19970602 <		
PRAI	DE 1996-19623744	19960614				
	WO 1997-EP2845	19970602				
os	MARPAT 128:75193					
GI						

Use of title compds. [I; Q1, Q2 = O, S; R1 = H, R11CO; R2 = R8R9NCO, AB R100CO, R11CO, R12SO2; R8 = H, alkyl, cycloalkyl, (substituted) aryl, heteroaryl; R9 = H, alkyl; R8R9N = (substituted) heterocyclyl; R10 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl; R11 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, aralkyl, heterocyclyl; R12 = alkyl, aryl, heterocyclyl; R1R2 = CR13R14; R1R2N = (substituted) heterocyclyl; R13 = H, alkyl, alkenyl, cycloalkyl, (substituted) aryl, heterocyclyl; R14 = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heterocyclyl, alkoxy, dialkylamino; R13R14 = cycloalkylidene; R3, R4 = OH, alkoxy, alkenyloxy, alkynyloxy, aralkoxy, cycloalkoxy, cycloalkenyloxy, aryloxy, heterocyclyloxy, aralkylthio, SH, arylthio, amino, etc.; R5-R7 = H, halo, cyano, NO2, alkyl, alkoxy, alkylthio, haloalkyl, haloalkoxy, haloalkylthio] for combating pests is claimed. Thus, 3-nitrophthalic anhydride was heated with BuOH to give 88.1% 3-nitrophthalic acid 2-Bu ester. The latter was refluxed with DMF di-Me acetal in PhMe to give 92% 3-nitrophthalic acid 1-Me ester 2-Bu ester. This in H2O/THF was treated with Zn and HCl to give 82.4% 3-aminophthalic acid 1-Me ester 2-Bu ester. I at 100 ppm gave 82-98% control of Botrytis cinerea on beans.

IT 200709-28-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aminophthalic acid derivs. as pesticides)

RN 200709-28-0 HCAPLUS

CN Benzoic acid, 3-[[(6-chloro-3-pyridinyl)carbonyl]amino]-2-[(methylamino)carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ \hline & C - NH & & \\ \hline & C - NHMe & \\ \hline & \\ O & & \\ \end{array}$$

L10 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:667205 HCAPLUS

DN 127:262339

TI Novel Folding Patterns in a Family of Oligoanthranilamides: Non-Peptide Oligomers That Form Extended Helical Secondary Structures

AU Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew D.

- CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
- SO Journal of the American Chemical Society (1997), 119(44), 10587-10593

 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- Anthranilamide derivs. are used as the basis for a series of novel oligomers that fold into helical secondary structures in the solid state. When combined with pyridine-2,6-dicarboxylic acid and 4,6-dimethoxy-1,3-diaminobenzene subunits, oligoanthranilamides can be induced to take up a coiled conformation corresponding to two turns of a helix. X-ray crystallog, show that intramol, hydrogen bonding and π - π stacking interactions are important in stabilizing the extended helical structures. Furthermore, both exptl. and calculated 1H NMR methods indicate that related conformations are taken up by the oligomers in chloroform solution
- IT 196312-02-4P 196312-04-6P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystallog.; helical conformation of oligoanthranilamides)
- RN 196312-02-4 HCAPLUS
- CN Benzoic acid, 2,2'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenyleneiminocarbonyl-6,2-pyridinediylcarbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 196312-04-6 HCAPLUS
CN Benzoic acid, 2,2'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenyleneiminocarbonyl-6,2-pyridinediylcarbonylimino-2,1-phenylenecarbonylimino)]bis-, dihexyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

155138-99-1 IT

RL: PRP (Properties)

(helical conformation of oligoanthranilamides)

155138-99-1 HCAPLUS RN

Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-CN phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

196311-73-6P 196311-77-0P 196311-92-9P IT

196311-95-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of oligoanthranilamides)

196311-73-6 HCAPLUS RN

2-Pyridinecarboxylic acid, 6-[[[2-[[[2-(methoxycarbonyl)phenyl]amino]carbo CN nyl]phenyl]amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 196311-77-0 HCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-(methoxycarbonyl)phenyl]amino]carbonyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

RN 196311-92-9 HCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-[(hexyloxy)carbonyl]phenyl]amino]carbonyl]phenyl]amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 196311-95-2 HCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[2-[[[2-[(hexyloxy)carbonyl]phenyl]amino]carbonyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

$$O = C$$
 $O = C$
 $O =$

IT 196312-07-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (model; helical conformation of oligoanthranilamides)

RN 196312-07-9 HCAPLUS

CN 2-Pyridinecarboxamide, N,N'-[(4,6-dimethoxy-1,3-phenylene)bis(iminocarbonyl-2,1-phenylene)]bis-(9CI) (CA INDEX NAME)

L10 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:543532 HCAPLUS

DN 127:134690

TI Inhibitors of MAdCAM-1-mediated interactions and methods of use therefor

IN Schwender, Charles F.; Shroff, Hitesh N.

PA Leukosite, Inc., USA

SO PCT Int. Appl., 107 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN CNT 1

PATENT NO.						KIND DATE			-	APPLICATION NO.						DATE				
PΤ	WO 9725351				A2 19970717			WO 1997-US291						19970103 <						
	. N	<i>I</i> :	AL.	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,		
			DK.	EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,		
			T.K.	T.R.	LS	LT.	LU.	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NΖ,	PL,	PT,		

												TR,	TT,	UA,	UG,	US,	UZ,	VN,	
			,	•	,				RU,	•									
		RW:	KΕ,	LS,	MW,	SD,	SZ,	υG,	AT,	BE,	CH,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	
			IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	
			MR,	NE,	SN,	TD,	TG												
	US	6037	324			Α		2000	0314	1	US 1	996~	5827	40 .		19	9960	104	
	CA	2241	169			AA		1997	0717	(CA 1	997-	2241	169		19	9970	103	<
	AU	9722	415			A1		1997	0801	i	AU 1	997-	2241	5		19	9970	103	<
	AU	7216	15			B2		2000	0713										
	ΕP	8716	70			A2		1998	1021]	EP 1	997-	9055	54		19	970	103	<
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	FΊ	•		•					•	•		•				
	JP	2000	5032	03		Т2		2000	0321		JP 1	997-	5253	31		19	9970	103	
	US	6274	556			В1.		2001	0814	1	US 1	998-	1098	79		19	9980.	702	
	US	2002	1031	11		A1		2002	0801	Ţ	JS 2	001-	8592	14		20	010!	516	
PRAT	US	1996	-582	740		A2		1996	0104										
		1997				W		1997	0103										
		1998						1998											
os		RPAT							J .										

AB The present invention provides novel compds. comprising peptide sequences which mimic the conserved amino acid motif LDTSL of MAdCAM-1 and which have groups bonded to the N- and C-termini. Also provided are methods of inhibiting the interaction of a cell bearing a ligand of MAdCAM-1, such as human $\alpha 4\beta 7$, with MAdCAM-1 or a portion thereof (e.g., the extracellular domain), comprising contacting the cell with a compound of the present invention. The MAdCAM-1 inhibitors are useful for treating disease associated with leukocyte infiltration of tissue, such as inflammatory bowel disease, with fewer side effects in other tissues where adhesion is mediated by $\alpha 4\beta 1$ integrin, for example. The inhibitors can also be used for induction of antibodies selectively bind epitopes of MAdCAM-1 and useful for quantitating MAdCAM-1 on cell surface.

IT 193218-88-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptide inhibitors of MAdCAM-1-mediated interactions for treating disease associated with leukocyte infiltration)

RN 193218-88-1 HCAPLUS

CN L-Threonine, N-[2-[(3-isoquinolinylcarbonyl)amino]benzoyl]-L-leucyl-L- α -aspartyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN AN 1996:446492 HCAPLUS

DN 125:167496

TI Oligoanthranilamides. Non-Peptide Subunits That Show Formation of Specific Secondary Structure

AU Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew D.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO Journal of the American Chemical Society (1996), 118(32), 7529-7541

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

GΙ

AB A family of novel oligomers based on the anthranilamide nucleus has been prepared and shown to form well-defined secondary structural features. H NMR and X-ray crystallog. techniques have demonstrated that intramol. hydrogen bonds play a key role in stabilizing both linear sheet and helical conformational forms. An example compound is the oligomeric anthranilamide I.

Ι

IT 155138-99-1P 155139-01-8P 180133-05-5P 180133-06-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and secondary structure determination of oligomeric anthranilamides)

RN 155138-99-1 HCAPLUS

CN · Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 155139-01-8 HCAPLUS
CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 180133-05-5 HCAPLUS CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[(phenylamino)carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 180133-06-6 HCAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[(phenylamino)carbonyl]phenyl]-, 1-oxide (9CI) (CA INDEX NAME)

L10 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:995215 HCAPLUS

DN 124:117098

TI Preparation of pyridylanilide derivatives as fungicides

IN Riordan, Peter Dominic; Boddy, Ian Kenneth; Osbourn, Susan Elisabeth

PA Agrevo UK Ltd., UK

SO PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

r FUN.	PATEN	IT NO.		KIN	DATE	; 		CATION NO.	DATE				
PΙ	WO 9525723				. 1995	0928	WO 1	995-GB570		19950316 <			
	N	•	•			FI,	HU, JP,	KR, KZ, MX,	NO,	NZ, PL, RO,			
	r	-	•	SK, UA,		DE	CH DE	DV FC FD	CD	CD IF IT			
	, r		•				•		•	GR, IE, IT, ML, MR, NE,			
			TD, T		22, 21,	20,	01, 00,	02, 011, 011,	J.,	112, 1111, 1121,			
	AU 95	18981		A1	1995	1009	AU 19	995-18981		19950316 <			
	AU 688473												
		EP 750611					EP 19	995-911403		19950316 <			
					. 1998								
			BE, C							NL, PT, SE			
		.43954								19950316 <			
		778				0228	HU 19	996-2547		19950316 <			
	HU 21	.4292		В		0302							
	BR 95	07105		Α	1997	0909	BR 19	995-7105					
	JP 09	P 09510471			1997	1021	JP 19	995-524455		19950316 <			
	AT 16	T 168099			1998	0715	AT 15	995-911403		19950316 <			
	ZA 95	02205		Α	1995	1031	ZA 1	995-2205		19950317 <			
	US 57	56524		Α	1998	0526	US 19	996-714149	-	19960918 <			
PRAI	GB 19	94-534	7		1994	0318							

WO 1995-GB570 MARPAT 124:117098 19950316

OS GI

$$R^{2}$$
 R^{2}
 R^{3}
 R^{3}

AB Title compds. I [X = 0, S; R1, R2 = H, alkyl, cycloalkyl, alkenyl, etc.; R3 = (substituted) pyridyl, pyrimidinyl, pyrazinyl, etc.] were prepared Condensation of 6-methoxynicotinoyl chloride with Me anthranilate in the presence of Et3N in THF afforded I (X = 0; R1 = R2 = H; R3 = 6-methoxy-3-pyridyl) which showed activity against barley powdery mildew, rice blast and apple scab at ≤ 500 ppm.

173055-91-9P 173056-05-8P 173056-17-2P 173056-21-8P 173056-46-7P 173056-75-2P 173056-88-7P 173056-95-6P 173056-96-7P 173056-97-8P 173057-04-0P 173057-19-7P

173056-97-8P 173057-04-0P 173057-19-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of anilide derivs. as fungicides)

RN 173055-91-9 HCAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxyamino)carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 173056-05-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxymethylamino)carbonyl]phenyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 173056-17-2 HCAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methoxymethylamino)carbonyl]phenyl]- (9CI) (CA INDEX NAME)

RN 173056-21-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[[(phenylmethyl)amino]carbonyl]pheny l]- (9CI) (CA INDEX NAME)

RN 173056-46-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-methoxy-N-[2-[(methylamino)carbonyl]phenyl]-(9CI) (CA INDEX NAME)

RN 173056-75-2 HCAPLUS

CN Carbamic acid, [2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

173056-88-7 HCAPLUS RN

3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]-6-methoxy- (9CI) (CA CN INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{MeO} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

173056-95-6 HCAPLUS RN

3-Pyridinecarboxamide, N-[2-[(diethylamino)carbonyl]phenyl]-6-methoxy-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & \parallel \\
 & C - NH \\
 & Et_2N - C \\
 & \parallel \\
 & O \\
\end{array}$$

RN 173056-96-7 HCAPLUS

Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, hydrazide (9CI) CN (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{N} \\ \end{array} \begin{array}{c} \text{H}_2\text{N} - \text{NH} - \text{C} \\ \text{O} \\ \end{array}$$

173056-97-8 HCAPLUS RN

Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, CN (1-methylethylidene)hydrazide (9CI) (CA INDEX NAME)

RN 173057-04-0 HCAPLUS

CN Benzoic acid, 2-[[(6-methoxy-3-pyridinyl)carbonyl]amino]-, 2-acetylhydrazide (9CI) (CA INDEX NAME)

RN 173057-19-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(4-chlorophenyl)amino]carbonyl]phenyl]-6-methoxy- (9CI) (CA INDEX NAME)

L10 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:858623 HCAPLUS

DN 123:256357

TI Preparation of anthranilic acid amide derivative as cyclic guanosine monophosphate-phosphodiesterase inhibitors

IN Ozaki, Fumihiro; Ishibashi, Keiji; Ikuta, Hironori; Ishihara, Hiroki; Souda, Shigeru

PA Japan

SO PCT Int. Appl., 204 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

î Mi	PAT	ENT NO.			KINI)	DATE		· AI	PLI	CATI	ON N	o.		DATE		
ΡI	WO	9518097			A1				WC			P226	2		19941	L 22 7	<
		W: AU	, CA,	CN,	FI,	HU,	KR,	NO,	NZ, E	RU, !	US TE	TT	T.H.	MC.	NL, PT,	. SE	
	CA	2155662		Cn,	AA		1995					1556		,	19941	1227	<
		9512824			A1				ΑU	J 19	95-1	2824			19943	1227	<
		694465			B2		1998 1995		FI	. 10	05-0	0399	۵		1994	1227	<
		686625 686625			A1 B1		1999		E-1	1.5	93-3	,0333	,		1331.	,22,	`
			, BE,	CH,		DK,	ES,	FR,	GB, G	GR,	IE,	IT,	LI,	LU,	MC, NL	, PT,	, SE
	CN	1118595	1		Α		1996	0313	Cì	1 19	94 - 1	9131	1		1994		
	JP	0818856	3		A2		1996	0723	JI	2 19	94-3	33692	0		1994		
	HU	74450			A2		1996	1230			-	2512		,	1994		
	RU	2128644			C1		1999	0410	RI	J 19	95-1	L2019	4		1994	L227	<

10/698,643

	AT 180468	E	19990615	АТ 1995-903999	19941227 <
	FI 9503968	Α	19951019	FI 1995-3968	19950823 <
	NO 9503305	Α	19951025	NO 1995-3305	19950823 <
	us 5716993	Α	19980210	US 1995-507476	19950914 <
PRAI	JP 1993-347092	Α	19931227		
	JP 1994-299110	Α	19941109		
	WO 1994-JP2262	W	19941227		
os	MARPAT 123:256357		,		Α.
GT					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Anthranilamide derivs. [I; R1, R2, R3, R4 = H, halo, OH, (halo)alkyl, AΒ (halo)alkoxy, nitro, hydroxyalkyl, cyano, (CH2)pNR9R10, S(O)qR13, (un)protected CO2H, (un)substituted tetrazolyl, CONH2, pyrazolyl, or imidazolyl; or adjacent two substituents selected from R1 - R4 together with the C atoms bonded to them forms a ring; wherein R9, R10 = H, (halo)alkyl, arylalkyl, heteroarylalkyl, acyl, (un)protected CO2H; or NR9R10 forms a ring; p = 0, 1-6; R13 = H, (halo)alkyl; q = 0, 1-2; R5, R6 = H, halo, OH, cyano, (halo)alkyl, (halo)alkoxy; or R5 and R6 together with the C atoms bonded to them form cycloalkane, oxolane, 1,3-dioxolane, or 1,4-dioxane ring; W = N, CH; R7, R8 = H, (halo)alkyl; or R1 and R7 together with the C atoms bonded to them form a ring optionally containing other N, O, or S atom; A = H, (halo)alkyl, X(CH2)mZ; wherein X = CO, CS, CH2, SO2; Z = OH, (halo) alkoxy, cyano, halo, etc.; Y = O, S; n = 0, 1-6] or pharmacol. acceptable salts thereof are prepared These compds. are useful for the treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and asthma. Thus, 2-nitro-5-chlorobenzoic acid was refluxed with SOC12 in benzene for 4 h and concentrated to give 2-nitro-5-chlorobenzoyl chloride which was amidated with piperonylamine in the presence of Et3N in THF to give a benzamide (II; R = NO2). This compound was reduced by Fe powder in a mixture of AcOH, H2O, and MeOH under gentle refluxing to give, after concentration and treatment with concentrated HCl in EtOH, N-piperonylanthranilamide derivative II. HCl (R

NH2). An anthranilamide derivative (III) showed IC50 of 0.4 nM against cyclic guanosine monophosphate-phosphodiesterase preparation from pig aorta.

1T 169043-36-1P 169043-37-2P 169044-06-8P 169044-07-9P 169044-08-0P 169044-09-1P 169044-10-4P 169044-11-5P 169044-56-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors)

RN 169043-36-1 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-chlorophenyl]- (9CI) (CA INDEX NAME)

RN 169043-37-2 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-chlorophenyl]- (9CI) (CA INDEX NAME)

RN 169044-06-8 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carb onyl]-4-cyanophenyl]- (9CI) (CA INDEX NAME)

RN 169044-07-9 HCAPLUS

CN 4-Pyridinecarboxamide, N-[4-bromo-2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & N \\ NH-C & N \\ C-NH-CH_2 & O \\ \end{array}$$

RN 169044-08-0 HCAPLUS

CN 4-Pyridinecarboxamide, N-[4-bromo-2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{O} & \text{N} \\ \text{NH-C} & \text{NH-CH}_2 \\ \text{O} & \text{OMe} \end{array}$$

RN 169044-09-1 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[[(3-chloro-4-methoxyphenyl)methyl]amino]carbonyl]-4-cyano-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN 169044-10-4 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromo-5-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN 169044-11-5 HCAPLUS

CN 4-Pyridinecarboxamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 169044-56-8 HCAPLUS

CN 4-Pyridinecarboxamide, N-[5-amino-2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-bromophenyl]- (9CI) (CA INDEX NAME)

Br
$$C-NH-CH_2$$
 NH C NH C NH C NH

L10 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:795361 HCAPLUS

DN 124:29779

TI 4-Aminoquinazoline derivatives as inhibitors of cGMP phosphodiesterase and TXA2 synthetase

IN Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.

PA Ono Pharmaceutical Co., Ltd., Japan

SO U.S., 42 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

PATENT NO. KIND DATE APPLICATION NO. DATE

ΡI	US 5439895	Α	19950808	US 1993-154691	19931119 <
	JP 06192235	A2	19940712	JP 1993-197039	19930714 <
	CA 2100626	AA	19940116	CA 1993-2100626	19930715 <
	AT 208771	E	20011115	AT 1993-305557	19930715
	ES 2167325	Т3	20020516	ES 1993-305557	19930715
	PT 579496	T	20020531	PT 1993-305557	19930715
	JP 08099962	A2	19960416	JP 1995-264667	19950920 <
	JP 2923742	B2	19990726		
PRAI	US 1992-913473	B2	19920715		
	US 1993-76431	В2	19930614		
os	MARPAT 124:29779				
GI					

$$(R^4)_n$$
 N
 $Z-CvB-(R^3)_m$
 I

or

as

AB The compds. of the formula I and acid addition salts thereof, salts thereof, and hydrates thereof wherein R1 is hydrogen or C1-4 alkyl; Y is C1-6 alkylene; A is ORO or S(O)pRO, in which RO is C1-4 alkyl-hydroxy; p is 0-2; Z is single bond, methylene, ethylene, vinylene or ethynylene; CyB is (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing

as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms, two

three nitrogen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atom, one nitrogen atom, (4) 4- or 5-membered, unsatd. or partially saturated, monocyclic hetero ring containing

hetero atoms, one, two or three nitrogen atoms, or (5) 4-7 membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,

one or two oxygen atoms, or one or two sulfur atoms; R3 = e.g., H, C1-4 alkyl, C1-4 alkoxy; R4 = e.g., H, C1-4 alkyl, C1-4 alkoxy; and m and n independently are 1 or 2; with the proviso that (1) a CyB ring does not bond to Z through a nitrogen atom in the CyB ring when Z is vinylene or

ethynylene, have inhibitory effect on cGMP-PDE, and addnl. on TXA2 synthetase. Thus, e.g., 2-(1-imidazoly1)-4-[2-(2-imidazoly1)-4-[3-(2-imidazoly1)-4-[3-(3-imidazol

hydroxyethoxy)ethyl]amino-6-ethynylquinazoline.2HCl (II.2HCl) (prepared by desilylation of a silylacetylene precursor) exhibited inhibitory effect on cGMP-PDE and TXA2 synthetase with IC50 = 4.6 + 10-8 M and 1.33 + 10-6 M, resp. Pharmaceutical formulations were given.

IT 157864-21-6P 157864-28-3P 157864-30-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(4-aminoquinazoline derivs. as inhibitors of cGMP phosphodiesterase and TXA2 synthetase)

RN 157864-21-6 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-5-fluorophenyl]- (9CI) (CA INDEX NAME)

RN 157864-28-3 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 157864-30-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-4-nitrophenyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:761961 HCAPLUS

DN 123:340173

TI 4-Aminoquinazoline derivatives as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase

IN Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.

PA Ono Pharmaceutical Co., Ltd., Japan

SO U.S., 44 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 5436233	Α	19950725	US 1993-154518	19931119 <
	JP 06192235	A2	19940712	JP 1993-197039	19930714 <
	CA 2100626	AA	19940116	CA 1993-2100626	19930715 <
	AT 208771	E	20011115	AT 1993-305557	19930715
	ES 2167325	Т3	20020516	ES 1993-305557	19930715
	PT 579496	${f T}$	20020531	PT 1993-305557	19930715
	JP 08099962	A2	19960416	JP 1995-264667	19950920 <
	JP 2923742	B2	19990726		
PRAI	US 1992-913473	B2	19920715		
	US 1993-76431	B2	19930614		
os	MARPAT 123:340173				
GI					

AB Title compds. I [R1 is H, C1-4 alkyl; Y is a single bond or C1-6 alkylene; A is (i) CyA-(R2)l, (ii) ORO or S(O)pRO in which RO is ROA or ROB; ROA is CyA-(R2)l; ROB is H or C1-4 alkyl; p is 0-2; CyA is, e.g., (1) 3-7 membered, saturated or unsatd., monocyclic carbocyclic ring, (2) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero

one nitrogen atom, one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero

one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms; R2 is R2A or R2B; R2A is, e.g., CF3, OCF3; R2B is, e.g., H, C1-4 alkyl, C1-4 alkoxy; Z is ZA or ZB, ZA is methylene, ethylene, vinylene, ethynylene; ZB is a single bond; CyB is, e.g., (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero

two or three nitrogen atoms, (3) 6-membered, unsatd. or partially saturated,

monocyclic hetero ring containing as a hetero atom, one nitrogen atom; R3 = e.g., H, C1-4 alkyl; R4 = e.g., NHSO2R11, R11 = e.g., C1-4 alkyl; l, m, n are independently 1 or 2 (with provisos)] are provided as inhibitors of cGMP-PDE and TXA2 synthetase. Thus, e.g., treatment of 2-(1-imidazolyl)-4-(2-methoxyethyl) amino-6-(2-triethylsilylethynyl) quinazoline (preparation given) with tetrabutylammonium fluoride afforded 6-ethynyl-4-(2-methoxyethyl) amino-2-(1-imidazolyl) quinazoline (II); II.2HCl demonstrated inhibition of cGMP-PDE with and TXA2 synthetase with IC50 = 4.6+10-8 and 2.4+10-6 M, resp. Pharmaceutical formulations were given.

IT 157864-21-6P 157864-28-3P 157864-30-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(4-aminoquinazoline derivs. as inhibitors of cyclic guanosine

3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase)

RN 157864-21-6 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-5-fluorophenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & O & F \\ \hline & C - NH & C - NH_2 \\ \hline & O & \\ \end{array}$$

RN 157864-28-3 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 157864-30-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-4-nitrophenyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:746792 HCAPLUS

DN 123:132021

TI Discovery of Potent Cyclic GMP Phosphodiesterase Inhibitors. 2-Pyridyland 2-Imidazolylquinazolines Possessing Cyclic GMP Phosphodiesterase and Thromboxane Synthesis Inhibitory Activities

AU Lee, Sung J.; Konishi, Yoshitaka; Yu, Dingwei T.; Miskowski, Tamara A.; Riviello, Christopher M.; Macina, Orest T.; Frierson, Manton R.; Kondo, Kigen; Sugitani, Masafumi; et al.

CS Biofor Inc., Waverly, PA, 18471, USA

SO Journal of Medicinal Chemistry (1995), 38(18), 3547-57 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB Moderate cyclic GMP phosphodiesterase (cGMP-PDE, PDE V) inhibitor 2-phenyl-4-anilinoquinazoline (I) was identified utilizing MultiCASE assisted drug design (MCADD) technol. Modification of I was conducted at the 2-, 4-, and 6-positions of the quinazoline ring for enhancement of cGMP-PDE inhibitory activity. The 6-substituted 2-(imidazol-1-yl)quinazolines are 1000 times more potent in in vitro PDE V enzyme assay than the well-known inhibitor zaprinast. The 6-substituted derivs. of 2-(3-pyridyl)quinazoline and 2-(imidazol-1-yl)quinazoline exhibited more than 1000-fold selectivity for PDE V over the other four PDE isoenzymes. In addition, 3 cGMP-PDE inhibitors were found to have an addnl. property of thromboxane synthesis inhibitory activity.

IT 157864-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyridyl- and imidazolylquinazolines as cyclic GMP phosphodiesterase and thromboxane synthesis inhibitors)

RN 157864-28-3 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

- L10 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
- AN 1995:714439 HCAPLUS
- DN 123:216778
- TI Metallohelices: Effects of Weak Interactions on Helical Morphology
- AU Kawamoto, Tatsuya; Prakash, Om; Ostrander, Robert; Rheingold, Arnold L.; Borovik, A. S.
- CS Department of Chemistry, Kansas State University, Manhattan, KS, 66506, USA
- SO Inorganic Chemistry (1995), 34(17), 4294-5 CODEN: INOCAJ; ISSN: 0020-1669
- PB American Chemical Society
- DT Journal
- LA English
- AB The significant effects of weak interactions on the morphol. of metallohelices are demonstrated in metal complexes of the helical ligand 2,6-bis[{(N'-acetophenoyl)anthranilamide}carboxyamide]pyridine (H2L). This ligand contains 2 aryl arrays that are held rigid through hydrogen bonds and covalently attached to a pyridyl diamidate metal binding chelate. The morphologies helixes formed with H2L results from the weak interactions between the appended arrays and the tridentate chelate. H2L has a helical structure in the solid state with the 2 appendage crossing, interacting through π -stacking: (P.hivin.1, a 7.3507(8), b 10.627(1), and c 20.098(3) Å; α 96.64(1), β 98.07(1), γ 90.26(1)°; V = 1543.6(3) Å3, Z = 2, 3598 unique data (Fo $\geq 4\sigma$ Fo), R(Rw) = 0.0523(0.0656)). NMR and IR studies on the diamagnetic NiL complex show that the helical structure is present in solution Structural studies by x-ray diffraction methods on the copper(II) derivs. of L2- show the large effects that coordination changes have on helical morphol. Two structural isomers were isolated for CuL: a five coordinate green compound (CuLg) and a four coordinate red complex (CuLr). The five coordinate green complex crystallized from toluene in the space group P.hivin.1 with two independent mols. in the asym. unit cell. The unit cell consts. are a 12.402(3), b 15.382(3), and c 23.267(5) Å, α 107.09(2), β 90.68(2), γ 104.18(2)°; V = 4096.4(15) $ilde{A}3$, and Z=4. Final residuals for the refinement of 985 parameters against 9210 data were R = 0.0678 and Rw = 0.0681 with a GOF = 1.96. four coordinate red complex crystallized from toluene in the space group C2/c with unit cell consts. a 24.087(6), b 12.165(3), and c 23.806 Å; β 117.450(2)°, and Z = 8. Final residuals for the refinement of 442 parameters against 2662 data R = 0.0411 and Rw = 0.0486 with a GOF = 0.95. The differences in these two structural isomers is even more pronounced in their crystal lattices where micropores dominate the lattice architecture for CuLg and extended helixes are present in CuLr.
- IT 168284-90-0
 - RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (crystal structure and complexation with copper and nickel)
- RN 168284-90-0 HCAPLUS
- CN 2,6-Pyridinedicarboxamide, N,N'-bis[2-[[(2-acetylphenyl)amino]carbonyl]phe nyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:71053 HCAPLUS

DN 122:105008

TI Intra- and intermolecular hydrogen bonding control of supramolecular structure

AU Hamilton, Andrew D.; Hamuro, Yoshitomo; Yang, Ji; Geib, Steven J.; Fan, Erkang

CS Department Chemistry, University Pittsburgh, Pittsburgh, PA, 15260, USA

NATO ASI Series, Series C: Mathematical and Physical Sciences (
1994), 426 (COMPUTATIONAL APPROACHES IN SUPRAMOLECULAR CHEMISTRY),
101-8

CODEN: NSCSDW; ISSN: 0258-2023

DT Journal

LA English

AB Hydrogen bonding is used to control supramol. structure in two distinct ways. The first involves intramol. hydrogen bonds to stabilize linear and helical conformations in synthetic oligomers. The second uses intermol. hydrogen bonding to direct the self-assembly of several interacting subunits.

IT 155138-99-1P 155139-01-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystallog. of)

RN 155138-99-1 HCAPLUS

CN Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 155139-01-8 HCAPLUS

CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:620104 HCAPLUS

DN 121:220104

TI Transition metal complexes of N-(2-benzamide)pyridine-2'-carboxamide, a potentially tridentate ligand containing one secondary and one primary amide group: preparation and characterization in the solid state

AU Manessi-Zoupa, E.; Perlepes, S. P.; Hondrellis, V.; Tsangaris, J. M.

CS Dep. Chem., Univ. Patras, Patras, Greece

SO Journal of Inorganic Biochemistry (1994), 55(3), 217-33 CODEN: JIBIDJ; ISSN: 0162-0134

DT Journal

LA English

The synthesis of N-(2-carbamoylphenyl)pyridine-2-carboxamide (LH2) is reported along with its employment as a ligand. [MCl2(LH2)2].DMF (M = Co, Ni), [Cu2Cl4(LH2)2].DMF, [CuCl2(LH2)2], [Co(OH)(LH)]n.nH2O, [M2(OH)2(H2O)x(LH)2] (M = Ni, Cu; x = 4, 2), [M(LH)2].xH2O (M = Ni, Cu; x = 0, 1), [Ni(H2O)2(LH)2].H2O, and [CuCl(LH)]n were isolated. The complexes were characterized by elemental analyses, conductivity measurements, x-ray powder patterns, thermal methods, variable-temperature magnetic susceptibilities, and spectroscopic (IR and far-IR, ligand field, ESR) studies. A variety of stereochemistries is assigned for the complexes in

the solid state. The neutral ligand acts as a bidentate chelating agent with ligated atoms being the ring N and the secondary amide O; the LH- ion behaves as a bidentate chelating Nring, Nsecondary amide or as a tridentate Nring, Nsecondary amide, Oprimary amide ligand depending mainly on the reaction conditions.

IT 157979-82-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of transition metal complexes)

RN 157979-82-3 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:605373 HCAPLUS

DN 121:205373

TI 4-aminoquinazoline derivatives, and their use as medicine

IN Lee, Sung Jai; Konishi, Yoshitaka; Macina, Orest Taras; Kondo, Kigen; Yu, Dingwei Tim

PA Ono Pharmaceutical Co., Ltd., Japan

SO Eur. Pat. Appl., 86 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 3

1711.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 579496	A1	19940119	EP 1993-305557	19930715 <
	EP 579496	B1	20011114		
	R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IE, IT, LI, LI	U, MC, NL, PT, SE
	JP 06192235	A2	19940712		19930714 <
	CA 2100626	AA	19940116	CA 1993-2100626	19930715 <
	AT 208771	E	20011115	AT 1993-305557	19930715
	ES 2167325	Т3	20020516	ES 1993-305557	19930715
	PT 579496	T	20020531	PT 1993-305557	19930715
	JP 08099962	A2	19960416	JP 1995-264667	19950920 <
	JP 2923742	B2	.19990726		
PRAI	US 1992-913473	Α	19920715		
	US 1993-76431	Α	19930614		
os	MARPAT 121:205373				
GI					

AB The title compds. I wherein R1 is H or alkyl; Y is bond or alkylene; A is (i) -CyAR2, (ii) -OR0 or -S(O)pR0, R0 = H, alkyl, etc., p is 0-2, (iii) -NR16R17, R16, R17 are H, alkyl; CyA is (1) a 3-7 membered monocyclic carbocyclic ring, (2) a 4-7 membered monocyclic hetero ring containing as hetero atoms, one N atom, one N and one O atoms, two N and one O atoms, or one N and two O atoms, (3) a 4-7 membered monocyclic hetero ring containing as hetero atoms, 1 or 2 O or S atoms, R2 is (1) H, (2) alkyl, (3) alkoxy, (4) -COOR5, in which R5 is H or alkyl, (5) -NR6R7, R6, R7 are H, alkyl, (6) -SO2NR6R7, (7) halogen, (8) CF3, (9) NO2 or (10) CF3O; Z is bond, methylene, ethylene, vinylene or ethynylene; CyB is a heterocyclic ring; R3 is H, alkyl, alkoxy, halogen or CF3; R4 is H, alkyl, alkoxy, etc., and acid addition salts thereof, salts thereof, and hydrates thereof were prepared and have inhibitory effect on cGMP-PDE, or addnl. on TXA2 synthetase. Thus, a representative prepared compound II had inhibitory activity IC50 of $3.6 \times 10-7$ on cGMP-PDE.

IT 157864-21-6P 157864-28-3P 157864-30-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of aminoquinazolines as cardiovascular agents)

RN 157864-21-6 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-5-fluorophenyl]- (9CI) (CA INDEX NAME)

RN 157864-28-3 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)phenyl]- (9CI) (CA INDEX NAME)

157864-30-7 HCAPLUS RN 3-Pyridinecarboxamide, N-[2-(aminocarbonyl)-4-nitrophenyl]- (9CI) (CA CN INDEX NAME)

L10 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

1994:323221 HCAPLUS AN

120:323221 DN

New molecular frameworks: formation of helical secondary structures in a ΤI group of oligoanthranilamides

Hamuro, Yoshitomo; Geib, Steven J.; Hamilton, Andrew D. ΑU

Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA CS

Angewandte Chemie (1994), 106(4), 465-7 (See also Angew. Chem., SO Int. Ed. Engl., 1994, 33(4), 446-8) CODEN: ANCEAD; ISSN: 0044-8249

DT Journal

LΑ German

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Helical oligoanthranilamide I (R = CO2Me) was prepared from 2,6-pyridinedicarbonyl dichloride and aminobenzamide derivative II (Y = NH2). II (Y = NH2) prepared from 2-nitrobenzoyl chloride condensation with anthranilic acid Me ester to give II, Y = NO2 followed by catalytic hydrogenation. I (R = CO2Me) was characterized by proton NMR and x-ray crystallog. and the nature of its helical structure discussed. Helical oligoanthranilamide III was also characterized by x-ray crystallog.

IT155139-01-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure and proton NMR of, conformational anal. in relation to)

155139-01-8 HCAPLUS RN

CN Benzoic acid, 2,2'-[(1-oxido-2,6-pyridinediyl)bis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

IT 155138-99-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal and mol. structure of)

RN 155138-99-1 HCAPLUS

CN Benzoic acid, 2,2'-[2,6-pyridinediylbis(carbonylimino-2,1-phenylenecarbonylimino)]bis-, dimethyl ester (9CI) (CA INDEX NAME)

- L10 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
- AN 1994:270304 HCAPLUS
- DN 120:270304
- TI 4-Hydroxy-2-quinolones. 18. Synthesis and antithyroid activity of 1-R-2-oxo-3-(4-oxo-3H-quinazolin-2-yl)-4-hydroxyquinolines
- AU Ukrainets, I. V.; Taran, S. G.; Bezugly, P. A.; Kovalenko, S. N.; Turov, A. V.; Marusenko, N. N.
- CS Ukr. Farm. Akad., Kharkov, 310002, Ukraine
- SO Khimiya Geterotsiklicheskikh Soedinenii (1993), (9), 1223-6 CODEN: KGSSAQ; ISSN: 0132-6244
- DT Journal
- LA Russian

GI

- AB Treating quinolinecarboxylates I (R = H, Me, Et, R1 = OEt) with anthranilamide gave 96-98% intermediate amides I (R1 = o-H2NCOC6H4NH) which underwent base catalyzed cyclization to give 95-96% quinazoline derivs. II. The latter could also be obtained starting from Et anthranilate derivative III. All compds. reduced the level of thyroxine with II (R = H) showing the greater decrease.
- TT 154325-54-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and intramol. cyclocondensation of, in preparation of
- (preparation and intramol. cyclocondensation of, in preparation of hydroxyoxoquinolylquinazolinone)
 RN 154325-54-9 HCAPLUS
- CN 3-Quinolinecarboxamide, N-[2-(aminocarbonyl)phenyl]-1,2-dihydro-4-hydroxy-2-oxo-(9CI) (CA INDEX NAME)

- L10 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
- AN 1982:162351 HCAPLUS
- DN 96:162351
- TI Anthranilic acid derivatives
- PA Kyoto Pharmaceutical Industries, Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 4 pp.
- CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN. CNT 1

r AIV.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	JP 56161362	A2	19811211	JP 1980-43744	19800403 <	
PRAI	JP 1980-43744		19800403	•		

OS CASREACT 96:162351

GΙ

AB Four anthranilic acid derivs. I (R = NO2, NH2, nicotinamido; R1 = Me, H), having smooth muscle-relaxing or contracting activity (no data), were prepared from Me 2-amino-3,4,5-trimethoxybenzoate (II). Thus, 2.45 g II acylated with 1.9 g 2-nitrobenzoyl chloride in CHCl3 gave 82% I (R = NO2, R1 = Me), which was reduced over Pd-C to give I (R = NH2, R1 = Me). Acylation with nicotinoyl chloride gave I (R = nicotinamido, R1 = Me) (III), which was hydrolyzed with 0.5 N NaOH at 40-50° to give I (R = nicotinamido, R1 = H). III was also prepared by cultivating Aspergillus terreus afficanus IFO 8835.

IT 81469-77-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 81469-77-4 HCAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-2-[[2-[(3-pyridinylcarbonyl)amino]benzoyl]a mino]-, methyl ester (9CI) (CA INDEX NAME)

IT 81469-76-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 81469-76-3 HCAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-2-[[2-[(3-pyridinylcarbonyl)amino]benzoyl]a mino]- (9CI) (CA INDEX NAME)

L10 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1980:586283 HCAPLUS

DN 93:186283

TI Some reactions of 2-heterocycle-4(3H)-quinazolinones with electrophilic reagents

AU Muraoka, Keiji; Ichikawa, Masataka; Hisano, Takuzo

CS Fac. Pharm. Sei., Kumamoto Univ., Japan

SO Yakugaku Zasshi (1980), 100(4), 375-85 CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

OS CASREACT 93:186283

GI

AB 2-(1-Oxido-2-pyridino)-3-phenyl-4(3H)-quinazolinone (I), 2-(1-oxido-2-pyridinio)-3-phenyl-4(3H)-quinazolinone 1-oxide, and the control compound, 3-phenyl-2-(2-pyridyl-4(3H)-quinazolinone (II) were nitrated under appropriate conditions to give 3-(3-nitrophenyl)-2-(1-oxido-2-pyridinio)-4(3H)-quinazolinone, 3-(3-nitrophenyl)-2-(1-oxido-2-pyridinio)-4(3H)-quinazolinone 1-oxide, and 3-(3-nitrophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone or the dinitro derivative 6-nitro-3-(3-nitrophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone selectively and in comparatively higher yield. II was halogenated with N-bromosuccinimide or N-chlorosuccinimide by varying reaction temperature and concentration of

H2SO4, and by adding silver sulfate as an activator, to give 3-(3-bromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone and 6-bromo-3-phenyl-2-(2-pyridyl)-4(3H)-quinazolinone or the dihalides 3-(3,4-dibromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone or 6-bromo-3-(3-bromophenyl)-2-(2-pyridyl)-4(3H)-quinazolinone, and a further derivative which was presumably a trihalide.

IT 75359-17-0 75359-18-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclization of)

RN 75359-17-0 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[(phenylamino)carbonyl]phenyl]- (9CI) (CF INDEX NAME)

RN 75359-18-1 HCAPLUS

CN 2-Pyridinecarboxamide, N-[2-[[(3-nitrophenyl)amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} R-C-NH & NO_2 \\ \hline \\ O & \end{array}$$

L10 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:546545 HCAPLUS

DN 79:146545

TI 2-Pyridyl-4(3H)-quinazolinones

IN Hisano, Takuzo; Ichikawa, Masataka; Ide, Hiroyuki; Noda, Kanji; Nakagawa, Akira; Motomura, Toshiharu

PA Hisamitsu Pharmaceutical Co., Inc.

SO Jpn. Kokai Tokkyo Koho, 7 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	0111 1				
-	PATENT NO.	KIND	DATE	DATE	
			~~~~~		
PI	JP 48062779 ·	A2	19730901	JP 1971-98092	19711203 <
	JP 54034749	B4	19791029		
PRAI	JP 1971-98092		19711203		
			1		

GI For diagram(s), see printed CA Issue.

AB Quinazolinones (I) were prepared by cyclizing, e.g., 2-nicotinamido-3'-chlorobenzanilide (II). Thus, heating II 18 hr at 200° gave I (R = m-Cl, pyridyl 3-substituted). Similarly, 18 addnl. I were prepared

IT 39122-37-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, pyridylquinazolinone from)

RN 39122-37-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(3-chlorophenyl)amino]carbonyl]phenyl](9CI) (CA INDEX NAME)

L10 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1973:58340 HCAPLUS

DN 78:58340

TI Syntheses and pharmacological activities of 2-heterocyclic substituted 4(3H)-quinazolinone derivatives

AU Hisano, Takuzo; Ichikawa, Masataka; Kito, Go; Nishi, Tomoyuki

CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SO Chemical & Pharmaceutical Bulletin (1972), 20(12), 2575-84 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

The preparation of a series of 2-pyridyl-4(3H)-quinazolinones is described. Studies on the structure-activity relationship demonstrated that 2-pyridyl, 3-pyridyl, and 4-pyridyl substitution at 2 position of quinazolinone ring, and o-, m-, and p-substitution of the aromatic ring at 3 position are suitable for manifestation of hypnotic activity. The order of potency of activities produced by the difference in the position of substitution of substituents at 2 and 3 position decreased in the order of 4-pyridyl, o-tolyl > 3-pyridyl, o-tolyl > 2-pyridyl, o-tolyl. The anthranilates of these 4(3H)-quinazolinones were inactive. A maximum hypnotic effect accompanied with other potent pharmacol. properties was observed in 2-(4-pyridyl)-3-o-tolyl-4(3H)-quinazolinone, the potency of which was equal to or stronger than Methaqualone in mice.

IT 39122-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 39122-37-7 HCAPLUS

CN 3-Pyridinecarboxamide, N-[2-[[(3-chlorophenyl)amino]carbonyl]phenyl]-(9CI) (CA INDEX NAME)

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ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
     1966:403958 HCAPLUS
AN
     65:3958
DN
OREF 65:699h,700a-f
TI
     Syntheses and reactions of imidazoles
ΑU
     Almirante, L.; Mugnaini, A.; Fritz, L. Polo; Provinciali, E.
CS
     Lab. Bioterapio Milanese Selvi, Milan
SO
     Bollettino Chimico Farmaceutico (1966), 105(1), 32-44
     CODEN: BCFAAI; ISSN: 0006-6648
DT
     Journal
LA
     Italian
OS
     CASREACT 65:3958
AB
     2-Aminopyridine (I) (425 g.), and 450 g. BrCH2CH(OMe)2 (II) in 500 ml.
     toluene refluxed 16 hrs. gave 1-(2,2-di-methoxyethyl)-2-aminopyridinium
     bromide, which was made basic in 400 ml. H2O to yield 322 g.
     1-(2,2-dimethoxyethyl)-2-imino-1,2-dihydropyridine (III), bl 108°;
     HCl salt m. 184-5° (EtOH). Similarly was prepared the 4-methyl
     derivative of III, b2 137%; picrate m. 147-8° (EtOH). III b2.5
     123-6^{\circ}, was also obtained from 19 g. I, 33.8 g. II, and 20.16 .
     NaHCO3 by boiling 25 hrs. in 40 ml. PhMe. By this method were prepared the
     6-methyl derivative of III, b1.5 120°, 2-imino-1-(2,2-
     dimethoxyethyl)pyrimidine, b2.5 123° [picrate m. 135-6°
     (EtOH)], and 1-(2,2-dimethoxyethyl)-2-imino-1,2-dihydrothiazole, b2
     112°; HCl salt m. 156-7° (iso-PrOH). III (322 g.) was added
     slowly to 1750 ml. H2SO4 at 0^{\circ} and the solution kept 5 hrs. at
     90° to give 203 g. imidazo[1,2-a]pyridine (IV), b0.5 97° [n]20D 1.6211; picrate m. 216-17° (EtOH). Similarly, 5-methylimidazo[1,2-a]pyridine, b1.5 109° [picrate m. 232-3°
     (EtOH)], 7-methylimidazo[1,2-a]pyridine b0.7 113° [picrate m.
     223-4° (EtOH)], imidazo[1,2-a]pyrimidine, m. 131-3° (C6H6),
     and imidazo[1,2-b]thiazole, b2 106° [picrate m. 205-6°
     (EtOH)], were prepared II (11.2 g.) in 11 ml. H2O containing 2.5 ml. 48% HBr
was
     shaken 2 hrs., poured into 150 ml. H2O, treated with 25 g. NaHCO3 and 8 g.
     5-bromo-2-aminopyridine, and shaken 7 hrs. at 20° to give 76%
     6-bromoimidazo[1,2-a]pyridine, b1.5 165°, m. 53-5°;
     perchlorate, m. 236-8° (EtOH). Similarly, 6-chloroimidazo[1,2-
     a]pyridine, b1.5 132° [perchlorate m. 223-4° (EtOH)] was
     prepared 2-Aminopyrimidine (19 g.), and 13.7 g. BrCH2OMe suspended in 80 ml.
     EtOH was heated 3 hrs. at 60° to give 29% 2-methylimidazo[1,2-
     a]pyrimidine hydrobromide, m. 254-5^{\circ}. Similarly, 2-methylimidazo[1,2-\alpha]pyridine b2 105° [HCl salt,
     195-6° (EtOH)], and 2,5-dimethylimidazo[1,2-\alpha]pyridine b0.5
     112° [perchlorate 215-16° (EtOH)] were obtained. IV (5.9
     g.) and 2.25 g. Me2NH in AcOH was mixed with 1.5 g. HCHO and 25 ml. AcOH,
     and heated 3 hrs. at 60° to give 6.7 g. hygroscopic
     3-(dimethylaminomethyl)imidazo[1,2-\alpha]pyridine, m. 80-1° (ligroine); methiodide m. 233-4° (EtOH). Similarly,
     2-methyl-2-(dimethylaminomethyl)imidazo[1,2-\alpha]pyridine-2HCl, m.
     250-1° (EtOH-Et2O) [methiodide m. 200-1° (decomposition) (EtOH)],
     2-methyl-3-(diethylaminomethyl)imidazo[1,2-α]pyridine-2HCl.H2O, m.
     203° (decomposition) (EtOH-Et2O), 2-methyl-3-(morpholinomethyl)imidazo
     [1,2-\alpha] pyridine, m. 93-5° (ligroine), 2-methyl-3-[4(\beta-
     hydroxyethyl)-piperazin-1-ylmethyl]imidazo [1,2-\alpha]pyridine, m.
     167-9^{\circ} (C6H6C6H12), 2-methyl-3-[bis-(2-
     hydroxyethyl)aminomethyl]imidazol, 2-α]pyridine, m. 114-16°
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(C6H6), 7-methyl-3-(dimethylaminomethyl)imidazo[1,2- $\alpha$ ]pyridine-2HCl, 250-2° (C6H6) [methiodide m. 232-3° (decomposition) (EtOH)], and 2-(p-chlorophenyl)-3-(di-methylaminomethyl)imidazo[1,2- $\alpha$ ]pyridine-2HCl, m. 222-4° (EtOH-Et2O), [methiodide m. 220-22° (decomposition) (EtOH)], were prepared IV (11.8 g.) in 20 ml. Me2NCHO was

with 46.5 g. POCl3 in 60 ml. Me2 NCHO with shaking at 0° and then heated 7 hrs. at 75° to give 31% 3-formylimidazo[1,2-α]pyridine, m. 127-9°; HCl salt 242.5-4.5° (EtOH).

The formyl derivative (66 g.), 39.5 g. H2NOH.HCl, and 65 g. HCO2Na in 500 ml. HCO2H was refluxed 3 hrs. with stirring to give 62 g. 3-carbamoylimidazo[1,2-α]pyridine, m. 252-5° (iso-PrOH); HCl salt m. 298-9°; perchlorate m. 257.5-9.5°. The carbamoyl derivative (62 g.) was suspended in 500 ml. POCl3 and refluxed 15 hrs. with stirring until clear to give 49.7 g. 3-cyanoimidazo[1,2-α]pyridine, m. 156.5-7.5° (iso-PrOH). This derivative (1.4 g.) in 30 ml. EtOH containing 4.3 g. 85% KOH in 8.6 g. H2O was refluxed 12 hrs. under N to yield 0.9 g. 3-carboxyimidazo[1,2-α]pyridine, m. 244-5° (decomposition) (H2O).

- RN 6188-07-4 HCAPLUS
- CN Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)- (7CI, 8CI) (CA INDEX NAME)

L10 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1966:403957 HCAPLUS

DN 65:3957

OREF 65:699f-h

TI New acyl derivatives of 4-aminoantipyrine

AU Dory, Istvan; Puklics, Maria

CS Chinoin Gyogyszer Vegyeszeti Termekek Gyara, Budapest, Hung.

SO Magyar Kemiai Folyoirat (1966), 72(4), 174-6 CODEN: MGKFA3; ISSN: 0025-0155

DT Journal

LA Hungarian

AB 4-Aminoantipyrine (I) and its Me-and PhCH2 derivs. were condensed with N-nicotinoyl o- and p-aminobenzoic acid, and, N-nicotinoylanthranilic acid (II), yielding compds. which have pain relieving properties, similar in activity to algopyrine and amidazophene, but of lesser toxicity. Thus the

Na salt of the nicotinoyl derivative in C6H6 or CH2Cl2 was treated with SOCl2 to yield the corresponding acyl halide, which without further separation, was condensed with I or its derivs. Compds. prepared include 4-[p-(nicotinoylamino)benzoyl] aminoantipyrine (III), 55.4%; the p-(nicotinoylamino)benzoyl; p-methylamino analog 93.3%; the 4-N-Me derivative of III, the 4-N-benzyl derivative of III, 34.7.%; and 4- N- methyl-4 - N- nicotinoylanthranilylaminoantipyrine. Condensation of I with II yielded, owing to ring closure,  $2\text{-}(\beta\text{-}pyridyl)\text{-}3\text{-}(4\text{-}antipyrinyl)\text{-}4\text{-}quinazolone}$ , instead of the expected condensation compound

- IT 6188-07-4, Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)(preparation of)
- RN 6188-07-4 HCAPLUS
- CN Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)- (7CI, 8CI) (CA INDEX NAME)

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	166.52	480.55
DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
DISCOUNT AMOUNTS (FOR QUALIFITING ACCOUNTS)	ENTRY	SESSION
CA GURGOTTER PRIOR		
CA SUBSCRIBER PRICE	-23.10	-23.10

STN INTERNATIONAL LOGOFF AT 08:59:53 ON 15 NOV 2004

## 10/698,643

Na salt of the nicotinoyl derivative in C6H6 or CH2Cl2 was treated with SOCl2 to yield the corresponding acyl halide, which without further separation, was condensed with I or its derivs. Compds. prepared include 4-[p-(nicotinoylamino)benzoyl]aminoantipyrine (III), 55.4%; the p-(nicotinoylamino)benzoyl; p-methylamino analog 93.3%; the 4-N-Me derivative of III, the 4-N-benzyl derivative of III, 34.7.%; and 4- N- methyl-4 - N- nicotinoylanthranilylaminoantipyrine. Condensation of I with II yielded, owing to ring closure, 2-( $\beta$ -pyridyl)-3-(4-antipyrinyl)-4-quinazolone, instead of the expected condensation compound

IT 6188-07-4, Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)(preparation of)

RN 6188-07-4 HCAPLUS

CN Nicotinanilide, 2'-(antipyrinylmethylcarbamoyl)- (7CI, 8CI) (CA INDEX NAME)

=> log ySINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 480.55 FULL ESTIMATED COST 166.52 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -23.10 -23.10CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 08:59:53 ON 15 NOV 2004